MODELING SALTWATER UPCONING IN COASTAL AQUIFERS

By

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Dedicated to all my friends, especially,

Dodzi

Kafui

Beau

Kibibi

Edem

Erin

Creighton

. . .

Ety

Naneje

Little

Rosa

Wiliwily

Arden

"Mr. Wrong"

Yan

. . .

. . .

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LIST OF SYMBOLS

a_L longitudinal dispersivity

a_T transversal dispersivity

B thickness of the aquifer

BL thickness of the lower layer

BP thickness of the pumpage layer

BS thickness of the saltwater layer

BU thickness of the upper layer

B' thickness of the semi-confining layer on the top of the upper zone

c relative chloride concentration with respect to freshwater background chloride concentration

c* actual chloride concentration

$\tilde{D}$, $\tilde{D}'$ tensor of the hydrodynamic dispersion

D_{xx}, D_{xy}, D_{xz}, D_{yx}, D_{yy}, D_{yz}, D_{zx}, D_{zy}, D_{zz}

D'_{xx}, D'_{xy}, D'_{xz}, D'_{yx}, D'_{yy}, D'_{yz}, D'_{zx}, D'_{zy}, and D'_{zz}

} components of the hydrodynamic dispersion tensor

f subscript or superscript indicating freshwater (e.g., q_x^f is the specific discharge of freshwater in the x direction)

g gravitational acceleration

h_f height of freshwater above mean sea level (MSL), in a phreatic aquifer

h_s depth at which is situated the interface between the freshwater and the saltwater, referring to MSL as standard level

i, j, k — finite-difference indices for x, y, and z direction, respectively (unless otherwise specified)

K — hydraulic conductivity of the porous medium (K_x, K_y, K_z hydraulic conductivity in the x, y, z direction, respectively)

k — intrinsic permeability of the porous medium

KL, KP, KS, and KU — horizontal hydraulic conductivities in the lower, pumpage, saltwater, and upper zones, respectively

KLP_z — vertical hydraulic conductivity between the lower zone and the pumpage zone

KLS_z — vertical hydraulic conductivity between the saltwater zone and the lower zone

KPU_z — vertical hydraulic conductivity between the pumpage zone and the upper zone

K'_z — vertical hydraulic conductivity in the semi-confining layer on the top of the upper layer

L — distribution function of chloride concentration

L — subscript indicating that the variable is evaluated at the elevation Z_L

n — effective porosity

P — pressure

Q, Q_p — pumping rate

$\vec{q}$ — specific discharge vector

q_{x_i} — specific discharge in the x_i direction (i.e., q_x, q_y, q_z specific discharge in the x, y, and z direction, respectively)

q_{z_o} — vertical specific discharge at the elevation z_o

q_{z_L} — vertical specific discharge at the elevation z_L

R_f — freshwater subdomain

R_s — saltwater subdomain

S_o — specific storage coefficient of the porous medium

s — subscript or superscript indicating saltwater (e.g. q_x^s specific discharge of saltwater in the x direction

S_{oL}	specific storage coefficient in the lower zone
S_{oP}	specific storage coefficient in the pumpage zone
S_{oS}	specific storage coefficient in the saltwater zone
S_{oU}	specific storage coefficient in the upper zone
s	drawdown
sH	drawdown in the water table
sL	drawdown in the lower zone
sP	drawdown in the pumpage zone
sS	drawdown in the saltwater zone
sU	drawdown in the upper zone
t	time
$\vec{V}$	seepage velocity vector
V_x, V_y, V_z	components of the seepage velocity vector in the cartesian coordinates
w	source and/or sink term in the mass balance equations
x, y, z	directions of the cartesian coordinate axes
Z	elevation with respect to Z_o
Z_o	initial position of the saltwater front; origin of the vertical (Z) axis
Z_b	lower boundary of the transition zone; elevation of the saltwater front
Z_L	elevation of the top of the lower zone
Z_p	elevation of the top of the pumpage zone
Z_t	upper boundary of the transition zone; elevation of the top of the transition zone
ZDT	equivalent saltwater thickness (defined in Equation 4.83)
ξ	density ratio factor
α	coefficient relating chloride concentration to the water density

η	dimensionless elevation with respect to Z_b
γ_f	specific weight of freshwater
γ_s	specific weight of saltwater
Ω_p	pumpage zone
Ω_T	transition zone
Ω_u	upper zone
Γ_b	lower boundary of the saltwater domain
Γ_f	upper boundary of the water table
Γ_t	upper boundary of the freshwater domain
δ	thickness of the transition zone
ρ_f	density of freshwater
ρ_s	density of saltwater
μ	dynamic viscosity
ϕ	piezometric head
χ	flow direction

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MODELING SALTWATER UPCONING IN COASTAL AQUIFERS

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Saltwater upconing under freshwater producing wells is a classical result of underground water development in coastal regions. Traditional approaches to solving the upconing problem assume a sharp interface between the fresh and saline water. They suffer from a lack of coherence with the physical phenomenon which includes a transition zone between the two fluids and a non-negligible vertical flow below the well.

In the present study, efforts have been directed toward a better representation of the physical phenomenon. A transition zone has been represented between the freshwater and the saltwater, and the effect of partial penetration of the well has been considered, allowing the representation of vertical flow above and under the well. The governing equations of continuity, motion, and solute transport are solved simultaneously, subject to specific boundary conditions. The result is

the development of three-dimensional partial differential equations describing the drawdown distributions, the growth of the saltwater mound, the development of the transition zone, and the chloride distribution in the pumping region. These equations are formulated into a finite-difference numerical model which is solved using a three-dimensional ADI method.

The mathematical formulation of the model is well detailed so that it can be adapted to solving the upconing problem under various field conditions. The model accounts for a variety of the aquifer's physical conditions that occur in the field, such as homogeneous or non-homogeneous, isotropic or non-isotropic, and leaky or non-leaky. The model can easily be adapted to simulate water table conditions as well. The model has been verified using existing analytical solutions and field data.

While the model is specifically designed for simulating the saltwater upconing phenomenon, the approach used can easily be adapted to solving other groundwater transport problems.

CHAPTER 1
GENERAL INTRODUCTION

1.1 Statement of the Problem

Groundwater in Florida is the main source of water supply for municipal, agricultural, industrial, and domestic use. The lack of adequate quantities of water of suitable quality has become acute in some coastal areas of the state. Overdevelopment of most of Florida's coastal regions has permitted seawater to enter aquifers, making water from wells salty (Parker et al., 1955; Christensen et al., 1982). The presence of saltwater under freshwater in coastal aquifers cannot stop the exploitation of the freshwater needed by a continuously growing population in those overdeveloped areas. The management of groundwater in coastal regions should therefore be based on the most accurate and complete information possible, including the best prediction of the response of the groundwater system to any intervention. Saltwater upconing is the response of the groundwater system to pumping in regions where the freshwater is underlain by saltwater. The present study attempts to advance modeling of upconing as a response of coastal aquifers to pumping from the groundwater system.

1.2 Evolution of Concerns in Groundwater Hydrology

Man's concern with groundwater started centuries ago; but it is only about 300 years since Pierre Perrault, Edme Mariotte, and Edmond Halle set hydrology on its modern scientific way. However, groundwater

hydrology as a physical science began with the work of Henri Darcy (1803-1858). He studied the movement of water through a porous medium and developed the relationship between the water velocity and the characteristics of the porous medium conveying that water.

Looking back at the development of groundwater hydrology, one can observe that concerns were different at different stages of the development of human society. With the progress of economies and the growth of populations, water demand and water management have become complicated problems which water engineers have to solve.

In the first stage, groundwater study was characterized by the need for knowledge of the quantity of reserved water in the ground; groundwater was then considered in the general water balance only. In the second stage, the importance of groundwater as a natural resource became, to some extent, the motivation for the study of groundwater hydrology. Extensive exploitation of groundwater began where surface water could not meet the water demands of growing economies and an increasing population.

The third stage began with problems generated by an overexploitation of the groundwater in areas of important concentration of population. Most of those areas are coastal regions where saltwater intrusion puts a threat on the quality of underground water.

Generally speaking, the quantity of freshwater has been the leading factor of groundwater hydrology development during those three stages. In recent years, a fourth stage started with the leading factor being the quality of the underground water. The most important source of contamination of groundwater in coastal regions is the saltwater underlying the fresh groundwater. Matson and Sanford (1913) discussed the

presence of saltwater under the freshwater along the Keys and at different places on the mainland of southern Florida. Many reports, most of them from the U.S. Geological Survey and the Florida Geological Survey, concluded the presence of saltwater under most of Florida's coastal aquifers; see Sellards and Gunter (1913), Cooper and Stringfield (1950), and Parker et al. (1955). Since Drabe and Badon-Ghyben (1888), many investigations have been carried out to locate the extent of saltwater intrusion. However, little attention has been paid to the upconing problem on a small scale. Christensen et al. (1982) studied the potential of coastal groundwater to be contaminated; they developed a "sensitivity index" varying from 0.0 to 1.0, and giving the degree of susceptibility of the groundwater to be contaminated. Figure 1.1 shows the results of their investigations. A sensitivity index greater than 1.0 indicates an aquifer that can fulfill much of the water demands of a coastal or inland community; a sensitivity index smaller than 0.01 suggests an aquifer highly susceptible to saltwater contamination and no new pumping of such an area should be implemented.

The problem related to saltwater intrusion which groundwater engineers are now facing in coastal areas is no longer just to determine the extent of the intruded saltwater. They must also determine the best program of producing freshwater in areas underlain by saltwater without carrying too much salt and rendering the produced water too salty for use. The goal of the present work is to develop a model which will meet that need. The pumping region will be considered on a small scale so that the physical situation will be described as exactly as possible.

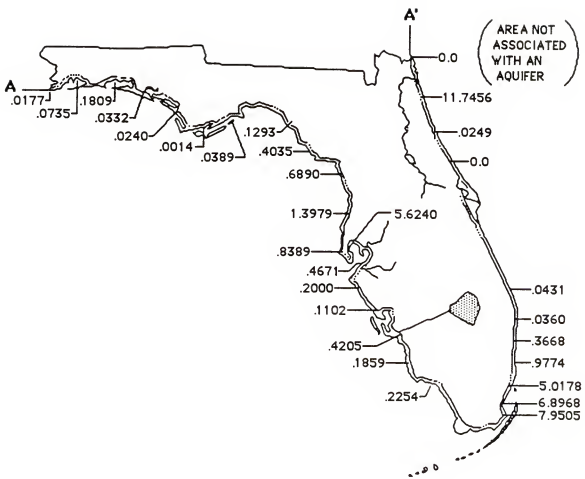


Figure 1.1 Sensitivity Index Along Florida's Coastline
(Source: Christensen et al., 1982)

1.3 Modeling Groundwater Systems

Physical, analog, and analytical models were used to simulate groundwater related problems, but their use was limited to simple applications. Todd (1960) and Bear (1979) give details and references on those models.

> A model may be defined as a simplified version of the real (here, groundwater) system that approximately simulates the excitation-response relations of the latter. The real system is very complicated and there is no need to elaborate on the need to simplify it.
>
> (Bear, 1985, p. 6)

In view of that statement, a model is a tool the groundwater hydrologist needs to simulate a management scheme and thus predict the response of the aquifer system to that management scheme.

The advent of digital computers brought the development of more sophisticated models which can describe very complex groundwater systems. Nonetheless,

> Numerical modeling of groundwater is a relatively new field which was not extensively pursued until the mid-1960's. Since that time, significant progress has been made in the development and application of numerical models for groundwater-related resource management. Management is here defined to include planning, implementation, and adaptive control of policies and programs related to the exploration, inventory, development, and operation of water resources containing groundwater. In spite of this progress, gaps still exist between the need for and the existence and actual use of groundwater models in management. The closing of these gaps can serve to improve the management of groundwater resources.
>
> (Bachmat et al., 1980, p. 1)

One of the most important gaps to be filled in groundwater-related problem studies is improved modeling of saltwater upconing under a single well or under a wellfield in coastal aquifers. Numerical models,

most of the time, are designed to be used by groundwater engineers whose knowledge of numerical methods and computer techniques is limited. The present work intends to present a numerical model which will be easily used by any groundwater engineer with limited background in numerical techniques.

1.4 Outline of the Work

The first chapter introduced the problem of saltwater intrusion and upconing in coastal aquifers. Chapter 2 presents the state-of-the-art of saltwater intrusion processes, including upconing under a well. The effect of a transition zone between freshwater and saltwater is discussed. A review of previous work in saltwater-related problems in coastal aquifers is presented. A brief review of the methods of solving contaminant transport in groundwater and partial penetration of wells ends the chapter.

The scope of the proposed work and the methodology used are presented in Chapter 3. The mathematical formulation of the upconing problem is presented in Chapter 4 while the resulting numerical model is developed in Chapter 5. The performance of the model is analyzed in Chapter 6. Chapter 7, finally, presents the conclusions and recommendations.

CHAPTER 2
BACKGROUND AND LITERATURE REVIEW

2.1 Saltwater Intrusion and Upconing Processes

Drabe and Badon-Ghyben (1888) and Herzberg (1901) found that saltwater occurs underground at a depth of about forty times the height of the freshwater above mean sea level (Figure 2.1). In a one-dimensional approach, they stated the hydrostatic equilibrium for a freshwater body floating on top of saltwater in unconfined aquifers in the northern coastal region of Europe. The assumptions on which they based their analysis can be summarized as follows:

(a) freshwater and saltwater are two immiscible fluids and they are separated by a sharp interface;

(b) a static equilibrium exists between the freshwater and the saltwater, so that the mass of a unit vertical column of freshwater extending from the water table to the freshwater-saltwater interface must have the same mass as the displaced saltwater, a column extending from the mean sea level (MSL) to the interface.

Using this information, Hubbert (1940) derived the Ghyben-Herzberg equation:

$$h_s = \frac{f}{s - f} h_f \qquad (2.1a)$$

or

$$h_s = \frac{f}{s - f} h_f \qquad (2.1b)$$

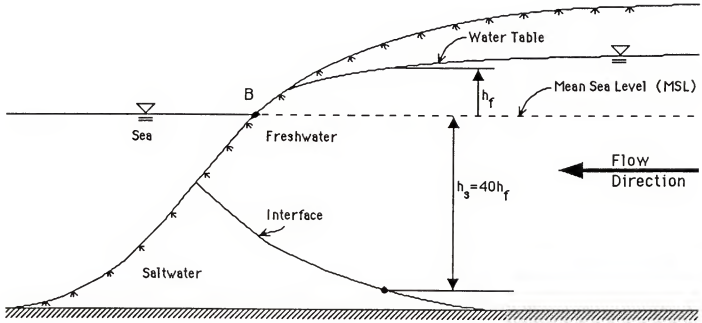


Figure 2.1 Interface Between Freshwater and Saltwater (Ghyben-Herzberg Theory)

where h_f = height of freshwater above MSL, in a phreatic aquifer

h_s = depth at which is situated the interface between the freshwater and the saltwater, referring to MSL as standard level

ρ_f = density of freshwater

ρ_s = density of saltwater

γ_f = specific weight of freshwater

γ_s = specific weight of saltwater

In regard to Equation 2.1, Hubbert (1940) noted,

> The assumption upon which the equation is derived is that we are dealing with a case of hydrostatic equilibrium, and to the extent that this assumption is valid the equation is strictly correct. In ground-water problems, however, the assumption is not valid at all, because the freshwater is not at constant potential but in a state of continuous motion. If no additional water were added by precipitation, the flow of the fresh water would continue until it had all been dissipated, and only saltwater with a water table at sea level would remain.
>
> We are therefore dealing with a dynamic equilibrium between flowing fresh water and static salt water . . .
>
> (Hubbert, 1940, p. 925)

It should be noted that for the saltwater to be under static conditions, it should be at constant potential. First the definition of the standard reference, under the circumstances, the MSL, contradicts that static state. In fact, the sea water level fluctuates around the mean sea level, implying that the potential in saltwater underground also fluctuates around a mean potential. Second, the assumption of the same potential of the freshwater and of the saltwater at the interface means that a variation of the potential in the freshwater along the interface implies a variation of the potential in the saltwater along the interface.

Ignoring for the time being the remarks just made and considering only the Hubbert (1940) assumption of a dynamic equilibrium between a flowing freshwater and a static saltwater, the sharp interface can be represented as shown on Figure 2.2.

It can be observed on Figure 2.2 that as the coastline is approached, the equipotential lines curve. Defining P'_a as the corresponding point of A along the potential τ_a, P_a the intersection of the vertical passing through A and the interface, the Ghyben-Herzberg equation underestimates the depth of the position of sharp interface near the coast, where the flow cannot be approximately considered horizontal.

In coastal aquifers, withdrawals from the freshwater zone reduce the effect of natural recharge, lowering therefore h_f, the height of the water table with respect to MSL. Consequently, the interface moves upwards and the toe moves inland: this process is called "saltwater intrusion." It implies inland movement of the seawater.

The saltwater intrusion phenomenon should not be confused with saltwater encroachment. Considering the coastline (point B on Figure 2.2) as the limit between the ocean and the land, the presence of seawater beyond point B is the encroachment of saltwater (literally speaking, saltwater being where it does not belong). This phenomenon can be considered the result or consequence of the process of saltwater intrusion. Factors which positively influence saltwater intrusion can be summarized as follows:

(a) drought over a relatively long period of time, lowering the water table, and therefore allowing the rise of the interface;

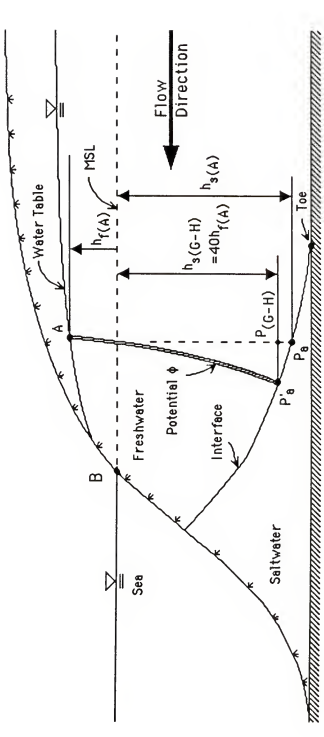


Figure 2.2 Groundwater Flow Near the Coast (Sharp Interface Theory)

(b) excessive withdrawals of freshwater as a consequence of increasing demand by municipalities, agriculture, and industries;

(c) excessive drainage reducing the infiltration from rainfall.

In overdeveloped coastal regions the infiltration from rainfall is usually reduced and the water demand is very high. Saltwater intrusion becomes a threat to the water supply of those regions. That is why many investigations have been devoted to the saltwater intrusion problem. Much effort has been made to stop the inland progression of seawater. Nevertheless, water demand in coastal regions is still growing and users have to rely on aquifers underlain by saltwater. The actual problem is to find out how to withdraw freshwater from these aquifers without getting salty water and without increasing the saltwater encroachment. The answer can be obtained through a numerical simulation of the aquifer on a small scale.

When water supply wells pump from a freshwater zone that is underlain by saltwater, there is a disruption of the pre-established equilibrium and of the potential distribution in the two layers; as a consequence the interface rises towards the pumping well (Figure 2.3). This phenomenon is called "interface upconing" (Bear 1979).

The effect of upconing cannot be well explained without modifying the theory of the sharp interface between freshwater and saltwater, for the two are miscible fluids and there exists a transition or mixing zone between them. The mixing process is controlled by the mechanism of dispersion (Bear 1972, 1979) and measured by what is termed the coefficient of dispersion. That coefficient is generally proportional to the water

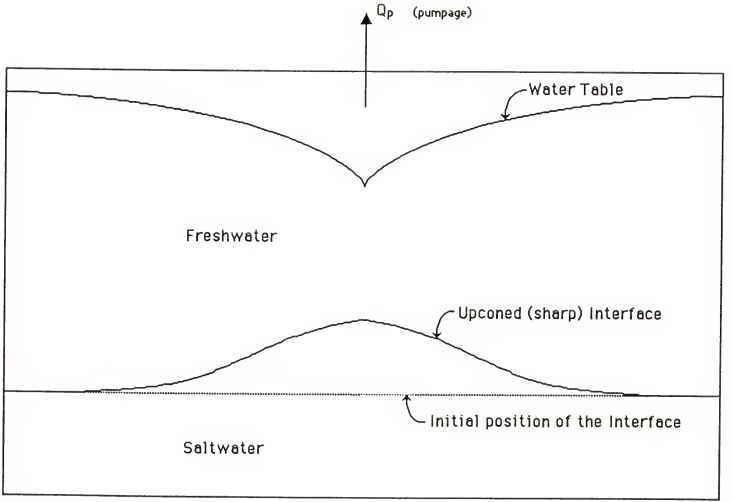


Figure 2.3 Upconed Interface Under a Pumping Well
(Sharp Interface Theory)

velocity in the porous medium. The theory of the sharp interface prevails where the thickness of the transition zone is negligible compared to the thickness of both the freshwater layer and the saltwater layer. Under a pumping well, the velocity of the water becomes important and so does the coefficient of dispersion. The thickness of the transition zone is no longer negligible under the pumping well; sometimes it is even thicker than the freshwater layer under the well. When pumping takes place in a coastal aquifer underlain by saltwater, the water comes from both the freshwater zone and the transition zone. When the pumping rate is high relative to the hydraulic characteristics of the aquifer, the transition zone becomes so important that its contribution makes the salt content of the pumped water become excessive.

Some attempts in modeling upconing which consider a transition zone between the freshwater and the saltwater have been made. While the importance of these works cannot be overestimated, they have fallen short of actually representing the physical situation, as will be seen in Chapter 3. A model designed to simulate a physical situation should describe as closely as possible that physical situation. On the other hand, as noted before, a spatial variation of the potential in the freshwater zone implies a spatial variation in the saltwater zone. As can be seen in Figure 2.4, the movement in the freshwater zone is mainly due to potential distribution. For the same reason, there is movement in the transition zone and so should it also be in the saltwater zone. Therefore, the assumption of static saltwater is not appropriate for the study of the upconing problem. Furthermore, in the analysis of "local problems," such as upconing under a well, the horizontal dimensions are

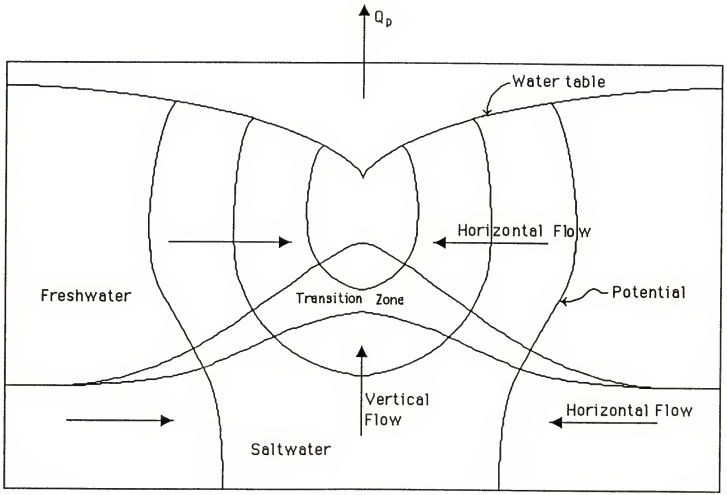


Figure 2.4 Upconing With Transition Zone Under a Pumping Well

comparable with the vertical ones and vertical flow components are significant around the well. Cooper (1959) already presented, "a hypothesis concerning the dynamic balance of fresh and salt water in coastal aquifer" (p. 461). He showed a possible way of considering the movement in the saltwater zone.

2.2 Methods of Solving Saltwater Intrusion and Related Groundwater Problems

In recent years, much attention has been paid to saltwater intrusion problems in coastal aquifers and numerous models have been developed to simulate the hydraulic physical behavior and the water quality in those areas. Nevertheless, there is no systematic classification of the existing models.

Bear (1979) made a survey of different ways of classifying models used to study groundwater flow problems. He first distinguishes between physical models (the sand-box model and the Hele-Shaw analog), and mathematical models (analytical and numerical models). He then presents the possibility of distinguishing between continuous models (or "models with distributed parameters") such as analytical models, physical and analog models of the type of Hele-Shaw model, and those with a discrete distribution of parameters (or lumped-parameter models) such as numerical models and resistance capacitance analogs. He also suggests the possibility of subclassifying the different classes presented above. Sa da Costa and Wilson (1979) suggest a more detailed classification of the existing models for studying saltwater intrusion problems in coastal aquifers. They first tried to include all the existing models in their classification; they also tried to subclassify the models according to

some characteristics well defined in their report. Bachmat et al. (1980) surveyed existing models in groundwater management and attempted a classification based on the purpose of the model, the water system treated, the level of spatial detail, and the management task which the model addresses. Their classification focuses mainly on numerical models and tends to be a guide in groundwater model selection; it is more specific than general. Javandel et al. (1984) distinguished "Analytical Methods," "Semianalytical Methods," and "Numerical Methods." Their classification considered exclusively contaminant-transport models in groundwater systems.

The present work considers two main groups of models: physical and mathematical models.

2.2.1 Physical Models

Physical models for saltwater intrusion problems are those based primarily on a physical representation of the aquifers. They are models of the types of sand box, Hele-Shaw, and electrical analogs. They are expensive to build and to calibrate. Usually, once built, they represent only one particular situation, which limits their use. With the advent of high-speed ditigal computers, the use of physical models has decreased considerably. Their current use serves as a form of comparison for the verification of a mathematical model. The group of physical models has been mentioned so far for the sake of completeness only. No further exploration of the classification of this type of model will be made. For more information, the reader is referred to Todd (1959) and Bear (1972, 1979).

2.2.2 Mathematical Models

Mathematical models represent the aquifer and its behavior by a set of differential equations. They can be classified according to the method used in solving those mathematical expressions by analytical, semi-analytical, and numerical models.

Analytical models are primarily based on finding an analytical function for a dependent variable, usually the potential, in terms of independent variables, generally space and time variables. The analytical function should satisfy both the known value of the dependent variable at boundaries or other points in the system and the differential equations. They generally give exact solutions to the considered problems, but the solutions are obtained for special cases of those problems (i.e., ideal cases obtained through several simplifying assumptions).

Numerical models are based on the discretization of the continuous time and space domain of the governing differential equations. This generally results in a series of simultaneous algebraic equations which are solved by the use of the computer.

Some mathematical models use both analytical and numerical techniques in the solution of groundwater flow and/or transport problems. Javandel et al. (1984) call them semianalytical models. However, they are not generally considered as a class in the literature. The reason for this can be assumed to be the possible confusion which might result in the distinction between analytical and semianalytical, since numerical integration is sometimes considered an analytical technique. In the present work, analytical and numerical models will be the two main classes of mathematical models to be considered. Among other

differences in the analysis of a groundwater system, analytical models consider the space and time domain as continuous and solve the basic differential equations analytically, while numerical models discretize the space and time domain to approximate the basic equations. Whenever a groundwater problem can be simplified and solved analytically, analytical models are preferred to numerical solutions. However, in the analysis of complex problems such as the upconing phenomemon under a multiple wells system, numerical solutions are preferred to analytical methods.

2.3 Analytical Models

The problem of saltwater intrusion in coastal aquifers was first investigated by Drabe and Badon-Ghyben (1889) and Herzberg (1901). Several authors then approached the problem with the more relevant situation where the movement in either one or both fluids has to be considered. According to De Josselin de Jong (1960), Lorentz (1913) was the first investigator to have given a correct account of how the movement of the fluids influences the behavior of the interface in a study of upconing of saltwater under a well. However, the problem of upconing did not get much attention at the beginning of saltwater intrusion investigations. Hubbert (1940) presented a general description of the flow of two fluids with different density, at either side of a steady interface between the two fluids.

Edelman (1940), using the method of flow nets, determined the shape and position of the sharp interface between a moving freshwater underlain by a static saltwater in a dune area adjacent to the sea. Several other investigators mathematically devised well-developed techniques for

the determination of the shape and position of the sharp interface when the freshwater flows over an assumed stationary saltwater body in coastal aquifers. Glover (1959) adapted a solution obtained by Kozeny (1953) for the flow of groundwater under gravity forces to the determination of the shape and position of the steady interface in coastal aquifers. Henry (1959, 1964a), Bear and Dagan (1964a), De Josselin de Jong (1965), Charmonman (1965), Verruijt (1968), Strack (1972, 1973, 1976) and Van der Veer (1977), using complex functions, conformal mapping and the hodograph techniques, derived several solutions for the steady state interface in coastal aquifers, considering different boundary conditions. Zaoui (1965) also solved the problem analytically in one dimension, but for the two-dimensional case, he transformed the differential equation in finite-difference schemes and used the Runge Kutta method for a numerical integration over the wedge of saltwater which was considered in movement. Those studies are two-dimensional models and they considered homogeneous and isotropic aquifers. Muskat (1937) and Rumer and Harleman (1963) performed laboratory experiments which confirmed those works.

Rumer and Shiau (1968), using the complex potential theory with the principle of superposition, solved the problem of the steady sharp interface for the homogeneous and isotropic and non-homogeneous and anisotropic cases. Their solution is valid for confined and unconfined aquifers when the length of the saltwater wedge is greater than the thickness of the aquifer. De Josselin de Jong (1960, 1969) used the method of singularity distributions to analyze multiple fluid flow through porous media. The concept as reported by De Josselin de Jong (1960) was first introduced in an unpublished study by Edelman in 1957,

"Grondwaterstroming van een niet homogene vloeistof." The technique consists of replacing different fluids with their own characteristics by one hypothetical fluid; rows of adequate singularities coinciding with the position of the interfaces between the fluids take care of the changes in properties among the fluids. Henry (1964) investigated the saltwater intrusion problem, considering vertical flow and dispersion at the interface of the two fluids. He considered a confined aquifer. De Josselin de Jong (1960) claimed also the possibility of the use of singularity distribution for the solution of the problem with a transition zone between the freshwater and saltwater.

Bear and Dagan (1964b) studied the movement of the sharp interface in a confined aquifer, using a vertically averaged flow equation in a two-dimensional model. They considered a dynamic seawater in this case, but they assumed that the interface remains abrupt while being displaced. They developed two expressions for the interface, one for an advancing wedge and the other for a retreating wedge. They also assumed that the movement of the interface is caused by a sudden change in the rate of seaward flow of freshwater only. They experimentally verified their work using a Hele-Shaw model. Curtis (1983) also analyzed the movement of the sharp interface using the distributed singularities method and he also verified his work using a Hele-Shaw model.

All of the above studies considered a steady state in the analysis of the seawater intrusion problem. Hantush (1968) derived an approximate time dependent differential equation which he solved analytically for different situations of the unsteady movement of the freshwater flow in an infinitely deep homogeneous and isotropic phreatic aquifer. In his solution, he also assumed that the interface remains sharp while

moving. In his study, the movement of the interface is in response to situations such as deep percolation from rainfall, artificial recharge, and seepage from irrigation water.

Todd and Huisman (1959) in a study to limit overdraft in the drinking water supply area of Amsterdam, applied Edelman's (1940) graphical method to determine the influence of recharge and pumping operation on the saltwater intrusion problem in coastal aquifers. Recently, several investigators, also using the sharp interface theory, have examined the effects of pumping and recharge wells on the saltwater intrusion problem in coastal aquifers. Bear and Dagan (1964a) investigated the cases of upconing toward a sink in an unbounded aquifer, upconing toward a sink in a confined aquifer of infinite thickness, and a drain above the interface in an aquifer of infinite depth. Strack (1976), using Girinskii's potential flow theory, solved the steady state interface problem for vertical wells in shallow coastal aquifers. Kishi and Fukuo (1977), in solving the same problem, transformed the saltwater region equation into a linear one which is continued to the equation in the freshwater region, resulting in a two-dimensional Poisson's equation applicable to the entire region. Assuming steady state conditions, the equations are then solved in integral form by using the method of Green's functions and the method of images. Kashef and Smith (1975) and Kashef (1976) analyzed the effects of pumping and/or recharge wells on the position of the sharp interface in shallow confined coastal aquifers, using the method of superposition and the Ghyben-Herzberg approximation.

Collins and Gelhar (1971) pointed out that little attention has been paid to the mathematical description of the multiple wedge

structure of the saltwater intrusion problem in coastal aquifers. They solved analytically the governing equations inland of the seawater wedge and used a numerical integration over the wedge. They also considered different situations of the semi-impervious layer dividing the aquifer system. However, they did not consider a leakage through the semi-impervious layer. They compared their work with a Hele-Shaw model study of Long Island, New York, which they had performed in 1970. Mualem and Bear (1974) looked at the Collins and Gelhar (1971) problem and considered a downward leakage through the semi-pervious layer. They also compared their results with laboratorty experiments with a Hele-Shaw model. Van der Veer (1976) gave solutions of some cases of non-steady interface in a nonhomogeneous anisotropic aquifer with multiple fluids flow. Hashish et al. (1979) considered a leaky layer at the top of the aquifer and analyzed the steady state position of the interface for different types of leakage and boundary conditions. Strack (1981a, 1981b), using potential theory and the singularity distributions methods, offered a two-dimensional model for solving the saltwater intrusion problem in the case of two infinite aquifers separated by a thin impervious layer and hydraulically connected. They included the nonhomogeneous and anisotropic cases; they also considered in their solution the effects of rainfall, creeks, canals, lakes, and wells.

Muskat (1946) empirically approximated the height of the cone beneath a well, considering a steady sharp interface between the freshwater and saltwater. Haubold (1975) modified Muskat's approximation to analyze the influence of the depth of penetration of the well on the interface position. He compared the results with interfaces determined experimentally in a Hele-Shaw model. His results concluded

that "changing the length of the producing interval of the well while keeping its pumping rate constant did not have a significant influence on the shape or position of the upconed interface" (Haubold, 1975, p. 254). The present investigation will show the deficiencies of Haubold's findings. Dagan and Bear (1968) analytically solved the problem of local interface upconing by the method of small perturbations. They also verified their results with a sand-box model. Schmorak and Mercado (1969) used field data to verify the Bear and Dagan solution. Rubin and Pinder (1977) analyzed the upconing phenomenon under a well and considered a transition zone between the freshwater and saltwater. They used the boundary layer integral method to develop an approximate expression for the thickness of the transition zone between the two fluids. Christensen et al. (1982) used Rubin and Pinder's model to establish a saltwater intrusion index in a study of saltwater intrusion in Florida's coastal aquifers. Volker et al. (1985) also using the boundary layer theory for the transition zone, adapted an analytical solution to the saltwater upconing on ocean atolls. They applied their method to study the influence of pumping and recharge on the boundaries of the mixing zone.

2.4 Numerical Models

In recent years, with the help of sophisticated computers, numerical methods have been used to solve complex equations, and to study coupled and uncoupled processes in heterogeneous and nonheterogenerous, isotropic and anisotropic groundwater systems. Problems that are too complicated to approach analytically have been successfully solved using numerical techniques. Nevertheless, the general tendency of the

investigators in dealing with saltwater intrusion is to greatly simplify the problem in order to reduce the computer time and cost. This attitude has reduced the capability of solving very complex saltwater related problems. Pinder and Cooper (1970) studied the movement of the transition between freshwater and saltwater in coastal aquifer systems. They solved the two-dimensional problem by considering both the equation of motion and the solute transport equation. The flow equation is a parabolic equation which is usually solved easily by finite-difference or finite-elements methods. The numerical approximation of the advective term leads usually to problems of inaccuracy and instability in the numerical scheme (Stone and Brian, 1963; Peaceman, 1977; Remson et al., 1971). In their analysis, Pinder and Cooper (1970) used a finite- difference approximation with the iterative alternating direction procedure to solve the steady state flow equation, while the method of characteristics and finite-difference approximation are used to handle advection and dispersion, respectively. Their solution yielded the steady state motion of the saltwater body and the distribution of salt concentration. However, they used a constant dispersion coefficient in the transport equation; and the variation in the flow is only due to changes in time of the solute concentration which affects the dynamics of the flow. Their model cannot therefore be qualified as unsteady or transient.

Segol et al. (1975) reconsidered the Pinder and Cooper problem. They used finite-elements for the space discretization and finite-difference for the time integration. They applied their model in a study of the Biscayne aquifer in south Florida.

Benedict et al. (1983) and Rubin and Rubin (1984) analyzed saltwater upconing in coastal aquifers. In their studies both the flow equation and the solute transport equation are solved using finite-difference approximations. They considered three different zones in each of which fluids of different density were considered. The boundary layer was used to represent the transition zone. While Benedict et al. (1983) assumed a stagnant saltwater, Rubin and Rubin (1984) considered the flow of the saltwater.

Shamir and Dagan (1971) and Polo and Ramos Ramis (1983), using the sharp interface theory in conjunction with the Dupuit assumption, analyzed the movement of the saltwater body as it responds to pumping and recharge stress on the aquifer system. Their solution was obtained using a finite-difference approximation. Shamir and Dagan (1971) verified their model with experimental results from a Hele-Shaw model. Fetter (1972) analyzed the steady state position of a sharp interface beneath oceanic islands. He developed a two-dimensional model using a finite-difference approximation along with the Dupuit assumption.

Sa da Costa and Wilson (1979) investigated the non-steady movement of the interface in both deep and shallow aquifers. They also used finite-elements to solve the problem in space, but used an implicit finite-difference approximation in solving the transient case.

Chandler and McWhorter (1975) investigated the behavior of a sharp interface under a pumping well. They used an implicit finite-difference approximation to solve the governing equations. They estimated the maximum well discharge obtainable without saltwater entrainment, assuming that the critical discharge is obtained when instability occurs at the interface.

Wirojanagud and Charbeneau (1983) analyzed both the steady state and transient behavior of the saltwater interface upconing under a well. They used a finite-elements method with an iterative scheme in solving the steady state model, and finite-elements in space and finite-differences in time in solving the transient model. They discussed criteria for establishing the permissible pumping rate and/or well depth.

Liu and Liggett (1978) considered an infinitely deep confined aquifer. They formulated and applied the boundary integral equations method (BIEM) to analyze the behavior of the sharp interface. Liu et al. (1981) extended the work by Liu and Liggett (1978) to deal with transient and non-linear interfacial boundary conditions.

2.5 Selection of the Approach to be Used in the Present Investigation

Analytical methods can only handle ideal cases of saltwater intrusion problems. The importance of numerical models lies in their capability of solving complex problems. In problems related to saltwater intrusion, existing numerical models fail to simulate actual upconing under a well because of simplifying assumptions introduced in those models.

None of the existing models can predict the salt content in water from wells over a certain period, while the most important decision variable in coastal aquifer system management is the salt content in the pumped water and its evolution over time. The best model to fully describe the upconing phenomenon is obtained by coupling the flow and solute transport equations in a fully three-dimensional model.

The optimum performance of such a model cannot be obtained without field experimentation. Therefore, the model should be easy to use. Pinder and Gray (1976) wrote:

> Because finite difference theory was well established and the methodology was generally known, this numerical scheme was the first to find widespread application in hydrology. . . . While the finite element approach has gained in popularity . . . there is a general reluctance on the part of practicing hydrologists to learn the fundamentals of finite element theory.
>
> (Pinder and Gray, 1976, p. 105)

Numerous groundwater models with different techniques of solution are currently available, but the most popular among users are those based on finite-difference techniques (Prickett and Lonnquist, 1971; Trescot et al. 1976). Even though the development of finite-elements methods, the method of characteristics, and the method of boundary integral equations were apparently due to the poor resolution of problems with distributed singularities by the finite-difference method, the latter still has a character of flexibility and easy understanding which makes its use readily acceptable by the users.

In the present work, numerical approximations of the governing equation will be made using finite-difference methods. Finite-difference methods for solving partial differential equations have been the subject of many books (Remson et al., 1971,). Also, experience shows that most first attempts at solving complex groundwater problems use finite-difference techniques (Pinder and Bredehoeft, 1968, and Prickett and Lonnquist, 1971). The apparent reason for the preference of the finite-difference method is its simplicity and flexibility.

Finite-difference methods, like other numerical methods, uses approximations, and their weakness is primarily in the accuracy of those

approximations. Nevertheless, the resulting inaccuracies can be made negligible through proper use of the methods. Furthermore, errors induced by the method may be outweighed by the inaccuracies due to the uncertainties in the specification of the aquifer's parameters.

CHAPTER 3
SCOPE AND METHODOLOGY OF THE PRESENT WORK

The chief objective of the present work is the development of a numerical model (UPCON) which simulates the upconing phenomenon under a producing well. The model will help in Florida's coastal aquifer management by predicting the evolution of the water contamination in a well tapping underground freshwater underlain by saltwater.

Since the mathematical model intends to simulate a physical system, the description and a good representation of the aquifer system become imperative. Any simplification or assumption will be dictated by the physical system and the problem under study. Figures 3.1 and 3.2 show, respectively, a plan and a cross-sectional view of a typical aquifer where the freshwater has been contaminated as a consequence of pumpage. Figures 3.2 through 3.4 show the spatial variability of the hydraulic characteristics of the aquifer. It is evident that the aquifer is neither homogeneous nor isotropic as is usually assumed in the literature where groundwater problems are solved analytically. The analysis of these figures suggests that the proposed model (UPCON) should consider the aquifer as non-homogeneous and non-isotropic. On the other hand, in the saltwater upconing analysis, the screened part of the well cannot extend over the whole thickness of the freshwater, for with that representation the well will pump saltwater from the start of its operation. The upconing analysis includes, therefore, partially penetrating

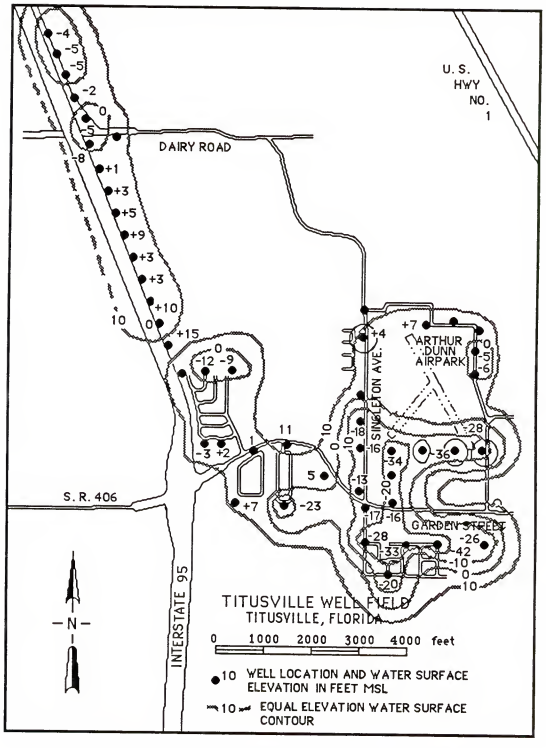


Figure 3.1 Potentiometric Heads in the Titusville Wellfield (Source: Reynolds, Smith and Hills, 1982)

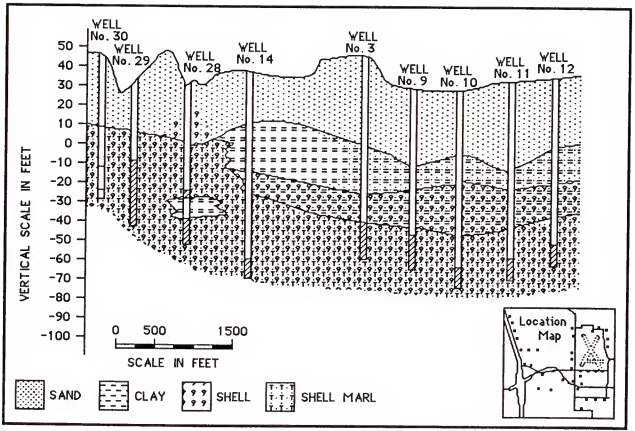


Figure 3.2 East-West Geologic Cross Section Through Titusville Wellfield (Source: Reynolds, Smith and Hills, 1982)

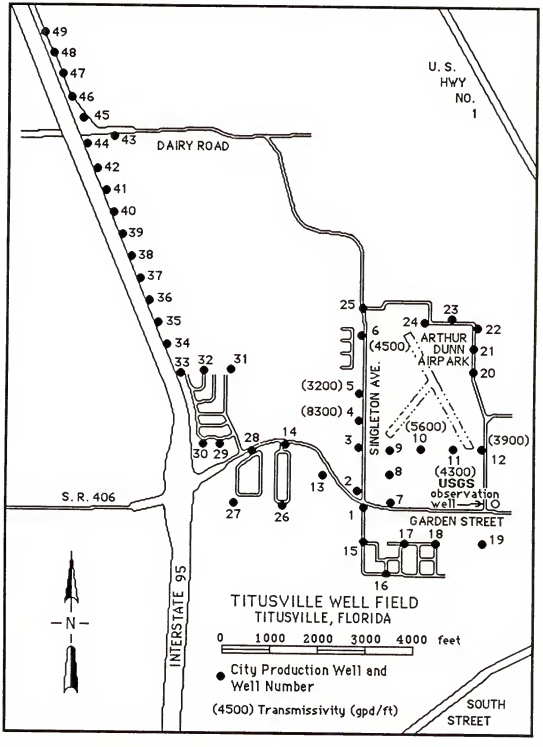


Figure 3.3 Estimated Transmissivity at Some Wells in Titusville Wellfield (Source: Reynolds, Smith, and Hills, 1982)

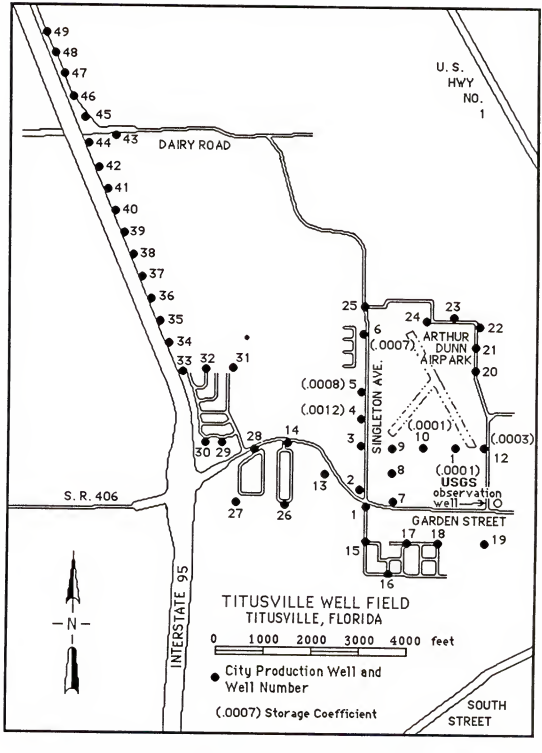


Figure 3.4 Estimated Storage Coefficient at Some Wells (Source: Reynolds, Smith and Hills, 1982)

well problems, and the vertical components of the flow cannot be neglected, at least near the well.

Figure 3.5 shows a schematic representation of the aquifer as an assemblage of cubical cells. Many wells can be in operation at the same time, but each of them is represented by a single cell. With that representation, the perturbation (the pumpage in the present case) affects a single cell and the behavior of the whole aquifer is dictated by the reaction of the surrounding cells in a horizontal plane, but also in a vertical plane. This representation holds when the interval of discretization (finite-difference grid size) is the same in all three directions x, y, z of the cartesian coordinates. In the present case, the well penetration and the original position of the fluids impose the vertical interval of discretization Δz. Figure 3.6 shows the conceptual representation of the cross-section of the aquifer. The zones represented are as follows:

1) The perturbed or pumpage zone, which is the thickness of the aquifer where the pumpage strongly affects the flow field in the aquifer. Its extent corresponds to the length of the screened part of the well.
2) The upper zone, which is the zone above the pumpage zone. The analysis of this zone will include eventual recharge or leakage from the water table on the top of the aquifer.
3) The lower or transport zone, which is the zone below the pumpage zone. It is the zone within which the vertical salt transport takes place in the form of the development and growth of a transition zone between the fresh and saltwater. Depending on the amount of salt coming from the saltwater zone

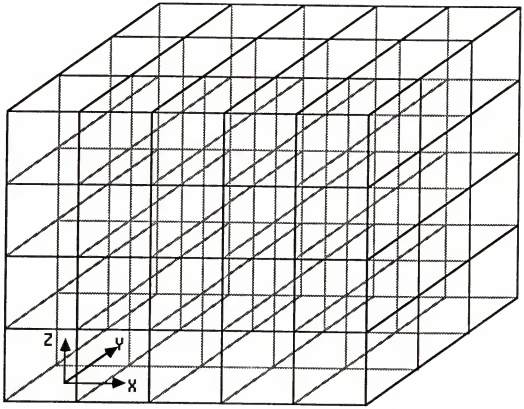


Figure 3.5 Conceptual Representation of an Aquifer

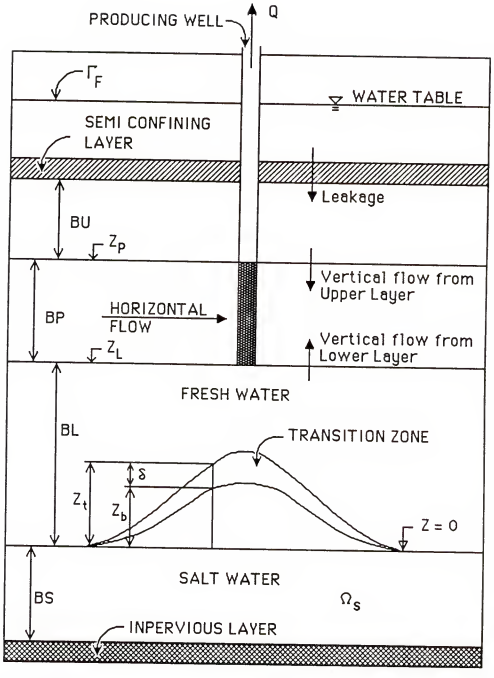


Figure 3.6 Conceptual Representation of a Cross-Section of a Coastal Semiconfined Aquifer with a Producing Well

and that being dispersed into the transition zone, a saltwater mound will form beneath the transition zone and above the saltwater zone itself.

4) The saltwater zone is below the transport zone. It represents the saltwater originally underlying the freshwater.

The approach used in the present study considers that the contamination of the well starts when the transition zone reaches the pumpage zone. Even though the space discretization in the vertical direction could be done in the usual manner, as in the horizontal directions, only those four zones are considered. The perturbation introduced by the pumpage in the flow field of the aquifer is a localized phenomenon, and the analysis of any undesirable effect produced by that perturbation depends on the way the localized phenomenon is handled in the model. It is therefore justifiable to consider the pumpage zone separately. Any further discretization may enhance the degree of resolution in the seepage velocity distribution, but this can be expected only if the variability in the aquifer characteristics is well known. Since the knowledge of aquifer's properties is usually limited to some sparse field data, average values obtained by considering the layers as shown on Figure 3.6 should be sufficient to describe the contamination of the aquifer.

Bear (1979) gives the three-dimensional governing equation for the flow and the solute transport. Assuming that the concerned fluids (the freshwater and the saltwater) are incompressible, the flow equation has been derived for each layer. The solute transport equation in the lower zone has been replaced by an alternate involving the thickness of the transition zone δ, and that of the saltwater mound, Z_b.

In a study of the transition zone between the freshwater and the saltwater, Rubin and Pinder (1977), using a boundary layer approach, developed an expression relating the chloride concentration in the lower zone to the thickness of the transition zone. That expression has been introduced into the transport equation which when integrated over the transport zone gives two equations for δ and Z_b. Chapter 4 presents the derivation of the mathematical model (flow and transport equations) of the upconing problem; Appendices A, B, and C give more details on some specific mathematical manipulations such as the integration of the transport equation.

The present study uses the finite-difference method for the solution of the governing equations of the upconing problem. The method of finite-difference approximation offers a simplicity and a flexibility which makes its use easy in practice.

Chapter 5 presents the derivation of the numerical model in terms of finite-difference equations. Standard finite-difference approximations of the differential equations have been used but a special scheme has been developed to handle the advective term in the transport equation. The approximation of advective terms by the finite-difference method usually leads to problems of accuracy and stability; it sometimes gives negative concentrations. The scheme used in the present study to approximate the advective term considers the flow directions, and a velocity direction tracking algorithm has been introduced into the model so that, depending on the direction of the flow, the proper approximation of the advective term is used. This approach greatly reduces the difficulties generally encountered in handling singularities when the

finite-difference method is used in solving groundwater transport problems.

A three-dimensional alternating direction implicit (ADI) scheme presented by Brian (1961) and Douglas (1962) has been adapted for the solution of the finite-difference equations of both the flow and the transport equations. The method converges and is very stable. Since the actual problem has not been treated analytically and therefore an exact solution does not exist at the present time, the accuracy of the method cannot be asserted. However, there exist some limiting cases for which analytical solutions have been developed (Bear and Dagan, 1968; Schmorak and Mercado, 1969). Chapter 6 discusses the verification of the model using the comparison of the numerical solution with those existing limiting cases. Also the model has been verified using actual field data.

Chapter 7 concludes the research work and gives recommendations for future work on the upconing problem.

CHAPTER 4
MATHEMATICAL FORMULATION OF THE UPCONING PROBLEM

The upconing problem is to be solved in a manner which is efficient in use of computer resources and at the same time maintains the integrity of the description of the physical system. This will be accomplished by schematizing the system based on physical processes and by simplification of the basic equations, especially by use of an integral method. This chapter presents details of these steps.

4.1 Geometry of the Problem and Assumptions

The schematization of the aquifer system is shown in Figure 4.1. A single well is used simply to describe the problem. Actually, many wells can be simultaneously pumping from the aquifer. The present problem involves two liquids separated by a transition zone, because of the density stratification between the freshwater and the saltwater. The flow region consists of two main subdomains: the freshwater subdomain R_f and the saltwater subdomain R_s, the two separated by the transition zone Ω_T.

The freshwater subdomain is bounded above by a semiconfining layer Γ_t; the saltwater subdomain is bounded below by a confining layer Γ_b. The boundary between the freshwater and the saltwater, the transition zone itself, is bounded by ideal surfaces, Z_t above and Z_b below. The lower boundary of the transition Z_b will be called "the saltwater

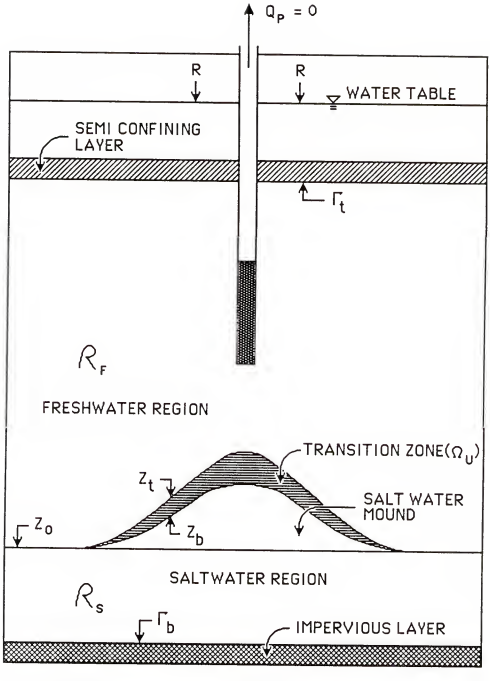


Figure 4.1 Geometry of the Saltwater Upconing Problem

front." The initial position of the saltwater front is assumed horizontal; its elevation is called Z_o.

The pumping rate from the well is Q and the infiltration and/or evapotranspiration (positive or negative recharge to the water table on the top of the upper boundary (Γ_t) of the freshwater subdomain) is R.

Ordinarily, the specification of the finite-difference grid is controlled primarily by boundary conditions. Here, the structure of the flow system in the problem of Figure 4.1 suggests a logical vertical subdivision of the aquifer system based on the differences in flow and transport behavior as one moves vertically in Figure 4.1. Figure 4.2 shows these subdivisions, which will form the vertical discretization for the numerical model and is described in the following sections.

1) The water table.

The water table is bounded above by a free surface Γ_F allowing recharge (infiltration) and/or loss (evapotranspiration). It is bounded below by a semiconfining bed through which leakage can occur. The water table in the present work is only considered for the completeness of the aquifer system. The only potentiometric head changes accounted for in the water table are due to loss or recharge rates.

2) The upper zone Ω_u.

The upper zone Ω_u is bounded above by the semi-confining layer and below by an imaginary surface of elevation Z_p which is defined by the elevation of the top of the screened portion of the well with respect to the initial position of the saltwater front Z_o. Flow in this zone is mixed, with strong vertical and horizontal components.

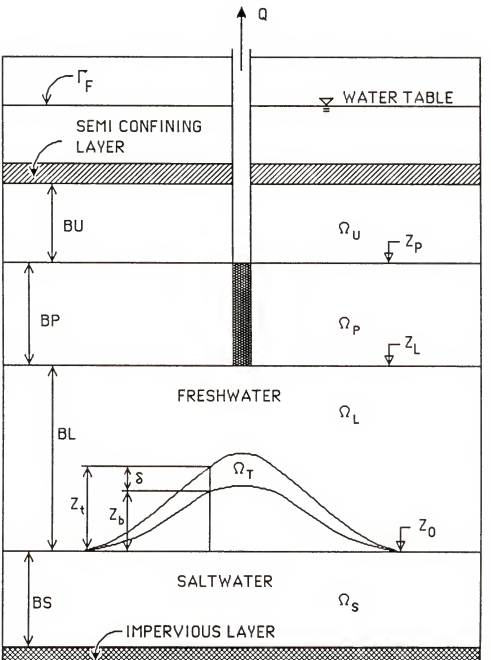


Figure 4.2 Vertical Subdivisions of the Aquifer System

3) The pumpage zone Ω_p.

The pumpage zone represents a layer of which the thickness corresponds to the screened portion of the well. It is bounded above by the surface Z_p and below by another imaginary surface Z_L which is defined by the elevation of the bottom of the screened portion of the well. The water withdrawal actually takes place in the pumpage zone. Flow in this layer is strongly horizontal.

4) The lower zone Ω_L.

The lower zone, or the "transport zone," is the layer between the pumpage zone and the saltwater zone. It is bounded above by the surface Z_L and below by the surface Z_o. When pumpage takes place in the pumpage zone, three distinct subregions can coexist in the lower zone: the saltwater mound between the surfaces Z_b and Z_o; the freshwater subregion between the surfaces Z_L and Z_t; and the transition zone where the chloride content goes from that of the saltwater at the saltwater front Z_b at the bottom of the transition zone to that of the freshwater at an ideal surface Z_t. The thickness of the transition zone δ is defined as the difference between the two surfaces Z_t and Z_b. Flow in the lower zone is also mixed; the specific discharge has horizontal and vertical components. In addition to the flow due to the potential distribution, there is a mass transfer (dispersion) between the saltwater and the freshwater due to the density variation in the lower zone.

5) The saltwater zone Ω_s.

The saltwater zone Ω_s corresponds to the original saltwater region R_s. It is bounded above by the surface Z_o, the original position of the saltwater front and below by a confining layer Γ_s. The chloride concentration in the saltwater zone is assumed to be constant everywhere

including Z_o. The flow in the saltwater zone also has horizontal and vertical components.

The subdivisions of the aquifer system as presented above fit the experimental configuration of the upconing phenomenon as presented by Pennink (1905) and shown on Figure 4.3.

The following are the assumptions considered in the analysis of the saltwater upconing in the present work.

1. The flow is three-dimensional.
2. The coordinate system considered is the cartesian one and coincides with the principal directions of the porous medium.
3. The freshwater and the saltwater are miscible fluids, each of which is homogeneous and incompressible in its own subdomain.
4. The porous medium is non-isotropic, non-homogeneous and elastic.
5. The viscosity of the freshwater and that of the saltwater are equal and constant.
6. The density ρ of the fluid is only a function of the chloride concentration c.
7. Flows in the transition zone and in the saltwater mound are completely defined by flow conditions in the lower zone.
8. The solute transport in the transition zone is totally controlled by "hydrodynamic dispersion in porous medium" (Bear 1972, 1979).
9. The dispersion coefficients are proportional to the seepage velocities.
10. The solute transport in the pumpage zone is purely advective (i.e., total mixing model).

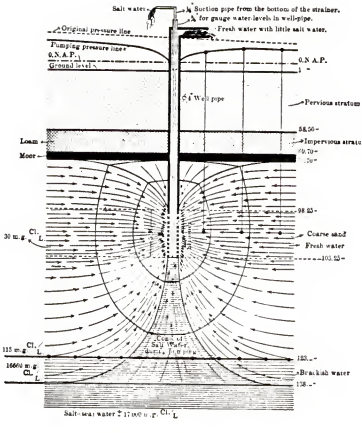


Figure 4.3 Cone of Saltwater Induced by Pumping Overlying Freshwater (From Pennink, J. M. K, Am. Soc. Civil Eng. Proc., Vol. 54, Pt. 4, p. 179, 1905. Reproduced with permission of the ASCE.)

4.2 Governing Equations

The basic equations used in the analysis of the saltwater upconing problem are the equations of continuity, motion, solute transport, and state.

4.2.1 Equation of Continuity

The general form of the equation of continuity (Bear, 1979) can be written as

$$\frac{\partial}{\partial x}(\rho q_x) + \frac{\partial}{\partial y}(\rho q_y) + \frac{\partial}{\partial z}(\rho q_z) + \frac{\partial}{\partial t}(n\rho) = 0 \qquad (4.1)$$

where

ρ = density of the fluid (ML^{-3})

n = effective porosity

t = time (T)

The components of $\vec{q}$ the specific discharge vector (LT^{-1}), are q_x, q_y, and q_z. When the density ρ is constant throughout the flow field, single phase flow case, Equation 4.1 reduces to

$$\nabla \cdot \vec{q} + \frac{\partial n}{\partial t} = 0 \qquad (4.2)$$

where

$$\nabla = \frac{\partial}{\partial x}\vec{i} + \frac{\partial}{\partial y}\vec{j} + \frac{\partial}{\partial t}\vec{k}$$

$\vec{i}$, $\vec{j}$, $\vec{k}$ = the unit vector in the x, y, z directions, respectively.

Equation 4.2 is the form of the continuity equation broadly used in groundwater literature. However, in the present study where the problem is one of flow of a variable density fluid, Equation 4.1 is a more appropriate form of the continuity equation.

4.2.2 Equation of Motion: Darcy's Law

The general expression of the Darcy's law is (Muskat, 1937; Hubbert, 1940; Bear, 1979):

$$q_\chi = -K_\chi \frac{\partial \phi}{\partial \chi} \tag{4.3}$$

where

q_χ = specific discharge in χ direction (LT^{-1})

K_χ = hydraulic conductivity in χ direction (LT^{-1})

ϕ = potentiometric head (L)

χ = direction of the flow (L)

The piezometric head ϕ is defined as

$$\phi = \frac{P}{\gamma} + Z \tag{4.4}$$

where

P = pressure at the considered point (FL^{-2})

Z = elevation of the considered point (L)

$\gamma = \rho g$ = specific weight of the fluid (FL^{-3})

g = gravitational acceleration (LT^{-2})

The hydraulic conductivity can be expressed as (Muskat, 1937; Hubbert, 1940; and Bear, 1979)

$$K_\chi = \frac{k_\chi}{\mu} \gamma \tag{4.5}$$

where

k_χ = intrinsic permeability of the porous medium in the χ direction (L^2)

μ = dynamic viscosity of the fluid (FTL^{-2})

In cartesian coordinates, Equation 4.3 can be written for each direction as follows:

x direction - $$q_x = -K_x \frac{\partial \phi}{\partial x} \tag{4.6a}$$

or

$$q_x = -\frac{k_x}{\mu} \gamma \frac{\partial \phi}{\partial x} \tag{4.6b}$$

y direction - $$q_y = -K_y \frac{\partial \phi}{\partial y} \tag{4.7a}$$

or

$$q_y = -\frac{k_y}{\mu} \gamma \frac{\partial \phi}{\partial y} \tag{4.7b}$$

z direction - $$q_z = -K_z \frac{\partial \phi}{\partial z} \tag{4.8a}$$

or

$$q_z = -\frac{k_z}{\mu} \gamma \frac{\partial \phi}{\partial z} \tag{4.8b}$$

x, y, and z are the directions of the cartesian coordinate axes.

About Darcy's law, Hubbert wrote

> The mechanical energy of the fluid per unit mass is, therefore, evidently the physical quantity we set out to find; and hereafter we shall refer to it as the potential of the fluid in question, there being as many distinct potentials as there are distinct fluids to be dealt with. (Hubbert 1940, p. 797)

Therefore, in the analysis of groundwater flow in coastal aquifers, it is common to write Darcy's law for the freshwater as

$$q_x^f = -K_x^f \frac{\partial \phi^f}{\partial x} = -\frac{k_x}{\mu^f} \gamma^f \frac{\partial \phi^f}{\partial x} \tag{4.9}$$

and for the saltwater as

$$q_x^s = -K_x^s \frac{\partial \phi^s}{\partial x} = -\frac{k_x}{\mu^s} \gamma^s \frac{\partial \phi^s}{\partial x} \tag{4.10}$$

where the superscripts f and s stand for freshwater and saltwater, respectively.

While this approach conforms to Hubbert's statement, it also leads to some confusion. In fact, the potential is the expression of the mechanical energy with respect of a specific fluid. When two neighboring fluid particles are in a dynamic equilibrium at a certain point,

their rate of movement should be equal. In the saltwater-freshwater literature, specifically in the theory of "sharp interface" between the freshwater and the saltwater, this condition is referred to as the "no-slip condition" at the interface, as shown in Figure 4.4. This means that at the saltwater-freshwater interface, oriented in the x direction

$$q_x^f = q_x^s \tag{4.11}$$

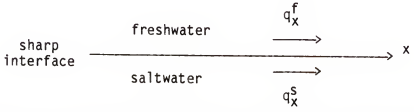


Figure 4.4 Freshwater and Saltwater Velocities at the Interface

Introduction of Equations 4.9 and 4.10 into Equation 4.11 leads to

$$\frac{\gamma^f}{\mu^f}\frac{\partial \phi^f}{\partial x} = \frac{\gamma^s}{\mu^s}\frac{\partial \phi^s}{\partial x} \tag{4.12}$$

and by assuming that $\mu^f \approx \mu^s$, Equation 4.12 becomes

$$\frac{\partial \phi^s}{\partial x} = \frac{\gamma^f}{\gamma^s}\frac{\partial \phi^f}{\partial x} \tag{4.13}$$

and

$$q_x^s = -K_x^s \frac{\gamma f}{\gamma^s}\frac{\partial \phi^f}{\partial x} = -K_x^f \frac{\partial \phi^f}{\partial x} \tag{4.14}$$

since

$$K_x^s = K_x^f \frac{\gamma^s}{\gamma^f} \tag{4.15}$$

Equation 4.14 suggests, therefore, that if the potential distribution of a fluid A is known under a given flow field condition, the

velocity distribution of a fluid B under the same flow field conditions can be studied using the known flow characteristics of the fluid A. The potential distribution of the fluid B can either be derived from fluid B velocity distributions (which are same as fluid A velocity distributions) using Darcy's law or from the potential distribution of fluid A using Equation 4.13.

However, the use of this technique, in order to be successful in the analysis of the mass conservation equation, should be associated with the mass of the concerned fluids, i.e.,

$$\rho^f q_x^f = -\rho^f K_x^f \frac{\partial \phi^f}{\partial x} \tag{4.16}$$

$$\rho^s q_x^s = -\rho^s K_x^f \frac{\partial \phi^f}{\partial x} \tag{4.17}$$

It should be emphasized at this point that the hypothesis of same flow field conditions only implies that the two fluids, when under that flow field condition, have the same velocity distributions. The above approximation can be considered valid as long as the components of the specific discharge q_x, q_y, and q_z are considered and the method of solution is the finite-difference approximation. Also, the saltwater zone is not stationary in the problem considered here.

The validity of Equations 4.16 and 4.17 can be explained in other ways, but since only their use matters in the present work, further explanation seems unnecessary.

4.2.3 Equation of Solute Transport

The general form of the solute transport equation can be expressed (Bear 1972, 1979) as follows:

$$\nabla \cdot (\vec{q} c^*) - \nabla \cdot (n\vec{D}' \nabla c^*) - \left(\begin{matrix}\text{source}\\ \text{rate}\end{matrix}\right) + \left(\begin{matrix}\text{sink}\\ \text{rate}\end{matrix}\right) = -\frac{\partial}{\partial t}(nc^*) \tag{4.18}$$

where

$\tilde{D}'$ = tensor of the hydrodynamic dispersion (L^2T^{-1})

c^* = concentration of constituent of interest

Many investigations have been carried out to define the expressions of the coefficients of the hydrodynamic dispersion. The following are the expressions suggested by Bear (1979) for the approximation of those coefficients:

$$D'_{xx} = a_T|\vec{v}| + (a_L - a_T)\, v_x^2/|\vec{v}| = [a_T (v_y^2 + v_z^2) + a_L v_x^2]/ |\vec{v}| \quad (4.19a)$$

$$D'_{xy} = D'_{yx} = (a_L - a_T)\, v_x v_y/ |\vec{v}| \quad (4.19b)$$

$$D'_{xz} = D'_{zx} = (a_L - a_T)\, v_x v_z/ |\vec{v}| \quad (4.19c)$$

$$D'_{yy} = [a_T(v_x^2 + v_z^2) + a_L v_y^2]/ |\vec{v}| \quad (4.19d)$$

$$D'_{yz} = D'_{zy} = (a_L - a_T)\, v_y v_z/ |\vec{v}| \quad (4.19e)$$

$$D'_{zz} = [a_T (v_x^2 + v_y^2) + a_L v_z^2]/ |\vec{v}| \quad (4.19f)$$

where

$$v_x = q_x/n \quad (4.20a)$$

$$v_y = q_y/n \quad (4.20b)$$

$$v_z = q_z/n \quad (4.20c)$$

$$|\vec{v}| = (v_x^2 + v_y^2 + v_z^2)^{1/2} \quad (4.21)$$

$\vec{v}$ = seepage velocity vector obtained from the specific discharge vector $\vec{q}$ which has components q_x, q_y and q_z in the x, y and z directions, respectively.

Defining

$$\tilde{D} = n\tilde{D}' \quad (4.22)$$

Equations 4.18 and 4.19 become

$$\nabla \cdot (\vec{q}c^*) - \nabla \cdot (D\nabla c^*) - \left(\frac{\text{source}}{\text{rate}}\right) + \left(\frac{\text{sink}}{\text{rate}}\right) = -\frac{\partial nc^*}{\partial t} \quad (4.23)$$

$$D_{xx} = [a_T(q_y^2 + q_z^2) + a_L q_x^2]/ |\vec{q}| \quad (4.24a)$$

$$D_{xy} = D_{yx} = (a_L - a_T)\, q_x q_y/ |\vec{q}| \quad (4.24b)$$

$$D_{xz} = D_{zx} = (a_L - a_T)\, q_x q_z/ |\vec{q}| \quad (4.24c)$$

$$D_{yy} = [a_T(q_x^2 + q_z^2) + a_L q_y^2]/ |\vec{q}| \quad (4.24d)$$

$$D_{yz} = D_{zy} = (a_L - a_T)\, q_y q_z/ |\vec{q}| \quad (4.24e)$$

$$D_{zz} = [a_T(q_x^2 + q_y^2) + a_L q_z^2]/ |\vec{q}| \quad (4.24f)$$

where

$$|\vec{q}| = (q_x^2 + q_y^2 + q_z^2)^{1/2} \quad (4.25)$$

4.2.4 Equation of State

The derivation of the equation of state is discussed in Appendix A. It can be expressed as follows:

$$\frac{\rho}{\rho_f} = 1 + \alpha\, (c^* - c_f^*) \quad (4.26)$$

or

$$\frac{\gamma}{\gamma_f} = 1 + \alpha\, (c^* - c_f^*) \quad (4.27)$$

where

ρ_f = density of freshwater

γ_f = specific weight of freshwater

c^* = chloride content in water of density ρ

c_f^* = chloride content in freshwater (i.e., background concentration)

α = coefficient relating the chloride concentration to the water density. The estimate of α is about 0.702.

The application of Equation 4.26 to saltwater yields

$$\frac{\rho_s}{\rho_f} = 1 + \alpha\,(c_s^* - c_f^*) \tag{4.28}$$

and defining ξ, which will be called the "density ratio factor" as

$$\xi = \alpha\,(c_s^* - c_f^*) \tag{4.29}$$

Equations 4.26 and 4.28, respectively, become

$$\frac{\rho}{\rho_f} = 1 + \xi\,\left(\frac{c^* - c_f^*}{c_s^* - c_f^*}\right) \tag{4.30}$$

and

$$\frac{\rho_s}{\rho_f} = 1 + \xi \tag{4.31}$$

The expression of the chloride concentration is easily obtained from 4.30 as

$$c^* = c_f^* + (c_s^* - c_f^*)\,\frac{\frac{\rho}{\rho_f} - 1}{\xi} \tag{4.32}$$

Rubin and Pinder (1977) suggested the following relation to describe the vertical distribution of the chloride concentration in the transition zone:

$$c^* = c_s^*\,L(\eta) \tag{4.33}$$

where

$$L(\eta) = 1 - 2\eta + \eta^2 \tag{4.34}$$

$$\eta = \frac{Z - Z_b}{\delta} \tag{4.35}$$

$$\delta = Z_t - Z_b \tag{4.36}$$

In the present work, $L(\eta)$ is what will be called the "influence function" of the vertical chloride distribution. In this work, δ is the thickness of the transition zone. In considering the general form of 4.32, Equation 4.33 has been modified into

$$c^* - c_f^* = (c_s^* - c_f^*)\, L(n) \tag{4.37}$$

so that

$$L(n) = \frac{c^* - c_f^*}{c_s^* - c_f^*} \tag{4.38}$$

Introduction of Equation 4.38 into 4.30 leads to

$$\frac{\rho}{\rho_f} = 1 + \xi\, L(n) \tag{4.39}$$

and subsequently

$$\frac{\gamma}{\gamma_f} = 1 + \xi\, L(n) \tag{4.40}$$

The expression of L(n) is discussed in Appendix B. The general form of L(n) can be expressed as

$$L(n) = \beta_0 + \beta_1 n + \beta_2 n^2 + \beta_3 n^3 + \cdots + \beta_n n^n \tag{4.41}$$

Hereafter, the expression $\frac{c^* - c_f^*}{c_s^* - c_f^*}$ will simply be written as $\frac{c}{c_s}$ with

$$c = c^* - c_f^* \tag{4.42}$$

$$c_s = c_s^* - c_f^* \tag{4.43}$$

where

c^* = actual chloride concentration

c_f^* = actual chloride concentration in the freshwater

c_s^* = actual chloride concentration in the saltwater

c = relative chloride concentration with respect to freshwater chloride content

c_f = 0

c_s = relative saltwater chloride content with respect to the freshwater chloride content

With those definitions, Equations 4.29, 4.30, 4.32, 4.37, and 4.38 become, respectively,

$$\xi = \alpha c \tag{4.44}$$

$$\frac{\rho}{\rho_f} = 1 + \xi \frac{c}{c_s} \tag{4.45}$$

$$c = c_s \frac{\frac{\rho}{\rho_f} - 1}{\xi} \tag{4.46}$$

$$c = c_s L(n) \tag{4.47}$$

$$L(n) = \frac{c}{c_s} \tag{4.48}$$

4.3 Development of the Flow Equations

The conceptual representation of the aquifer system was shown in Figure 4.2. The zoning only attempts to delineate the finite-difference grid size in the vertical direction of the cartesian coordinate. Since the problem is three-dimensional, the finite-difference elements might be referred to as finite-difference blocks as opposed to finite-difference grids for two-dimensional problems. The fluids are considered homogeneous (i.e., of constant density) in each finite-difference block of the considered zones, except in the finite-difference blocks which compose the lower zone. In the blocks of the lower zone, the density varies from that of the saltwater ρ_s at the lower boundary of the transition zone to that of the freshwater ρ_f at Z_t, the top of the transition zone. When the elevation of the top of the transition zone Z_t is greater than the top of the lower zone, Z_L, the surface Z_t becomes imaginary, because a total mixing is assumed in the pumpage zone. In

that case, the characteristic value of the density at the top of the lower zone can be defined as

$$\rho_L = 1 + \xi L(n_L) \tag{4.49}$$

where

$$n_L = \frac{Z_L - Z_b}{\delta} \tag{4.50}$$

δ - is still the difference between the imaginary value Z_t and the actual value of Z_b.

Adding source and/or sink term to Equation 4.1 and dividing by ρ_f (the freshwater density) yields

$$\frac{\partial}{\partial x}\left(q_x \frac{\rho}{\rho_f}\right) + \frac{\partial}{\partial y}\left(q_y \frac{\rho}{\rho_f}\right) + \frac{\partial}{\partial z}\left(q_z \frac{\rho}{\rho_f}\right) + \frac{\rho}{\rho_f} w(x,y,z,t) + \frac{\partial}{\partial t}\left(n \frac{\rho}{\rho_f}\right) = 0 \tag{4.51}$$

where

$w(x,y,z,t)$ = source and/or sink terms; it is positive for sinks and negative for sources

Bear (1979) shows that

$$\frac{\partial}{\partial t}(n\rho) = \rho S_{op} \frac{\partial P}{\partial t} + n \frac{\partial \rho}{\partial t} \tag{4.52}$$

where

$$S_{op} = \frac{1}{\rho g} S_{o\phi} \approx \frac{S_o}{\rho g} \tag{4.53}$$

S_o = specific storage coefficient of the aquifer (L^{-1})

$$\frac{\partial P}{\partial t} \approx \rho g \frac{\partial \phi}{\partial t} \tag{4.54}$$

The combination of Equations 4.51 through 4.54 gives

$$\frac{\partial}{\partial x}\left(q_x \frac{\rho}{\rho_f}\right) + \frac{\partial}{\partial y}\left(q_y \frac{\rho}{\rho_f}\right) + \frac{\partial}{\partial z}\left(q_z \frac{\rho}{\rho_f}\right) + \frac{\rho}{\rho_f} w(x,y,z,t) + \frac{\rho}{\rho_f} S_o \frac{\partial \phi}{\partial t} + n \frac{\partial}{\partial t}\left(\frac{\rho}{\rho_f}\right) = 0 \tag{4.55}$$

where the potential ϕ is defined with respect to freshwater as the fluid of reference.

Considering a point in the flow field where the change of the potential ϕ can be considered neglible and where the vertical specific discharge also is negligible, and defining the potential at that point as ϕ_o, the drawdown s at any point in the flow field can be defined as

$$s(x,y,z,t) = \phi_o - \phi(x,y,z,t) \tag{4.56}$$

so that

$$\frac{\partial \phi}{\partial x} = - \frac{\partial s}{\partial x} \tag{4.57}$$

and

$$q_x = + K_x \frac{\partial s}{\partial x} \tag{4.58}$$

Equation 4.55 then takes the form

$$\frac{\partial}{\partial x}(q_x \frac{\rho}{\rho_f}) + \frac{\partial}{\partial y}(q_y \frac{\rho}{\rho_f}) + \frac{\partial}{\partial z}(q_z \frac{\rho}{\rho_f}) + \frac{\rho}{\rho_f} w(x,y,z,t) + n\frac{\partial}{\partial t}(\frac{\rho}{\rho_f}) = S_o \frac{\rho}{\rho_f} \frac{\partial s}{\partial t} \tag{4.59}$$

Equation 4.59 represents the general form of the three-dimensional flow equation for the aquifer system as shown on Figure 4.2. However, referring to Figure 4.2, it can only be applied to a zone composed of finite-difference blocks in which the density is considered vertically constant. Here, since the density in the lower zone varies vertically, Equation 4.59 should be integrated from Z_o to Z_L to give the actual flow equation for that zone.

The horizontal specific discharges q_x and q_y have vertically averaged values within each finite-difference block ($\Delta x \cdot \Delta y \cdot \Delta z$). However, because of the vertical variation of the fluid density within each finite-difference block of the lower zone, it can be argued that q_x and q_y might also vary vertically. Then, a function g(z) can be derived

for representing that vertical variation so that the horizontal specific discharges would be

$$q_x(t) = G_x(x,y,z,t) \tag{4.60}$$

$$q_y(t) = G_y(x,y,z,t) \tag{4.61}$$

for each finite-difference block of the lower zone. In the present study, however, q_x and q_y are considered constant within each finite-difference block of the lower zone also. The integration of Equation 4.52 will then be carried out with the assumption of q_x and q_y being constant within each finite-difference block of the lower zone.

Introducing Equation 4.45 into 4.59 and considering the fact that $w(x,y,z,t) = 0$ in the lower zone leads to

$$\frac{\partial}{\partial x} q_x + \xi \frac{\partial}{\partial x}\left[q_x \frac{c}{c_s}\right] + \frac{\partial}{\partial y} q_y + \xi \frac{\partial}{\partial y}\left[q_y \frac{c}{c_s}\right] + \frac{\partial}{\partial z} q_z + \xi \frac{\partial}{\partial z}\left[q_z \frac{c}{c_s}\right]$$
$$+ \xi n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) = S_o \frac{\partial s}{\partial t} + \xi S_o \left(\frac{c}{c_s}\right) \frac{\partial s}{\partial t} \tag{4.62}$$

The integration of Equation 4.62 from Z_o to Z_L following the approach used in Appendix C gives

$$Z_L \frac{\partial q_x}{\partial x} + \xi \frac{\partial}{\partial x}\left[q_x\left(Z_b + \delta \int_o^{\eta_L} L(\eta)\, d\eta\right)\right] - \xi q_x L(\eta_L) \frac{\partial Z_L}{\partial x}$$

$$+ Z_L \frac{\partial q_y}{\partial y} + \xi \frac{\partial}{\partial y}\left[q_y \left(Z_b + \delta \int_o^{\eta_L} L(\eta)\, d\eta\right)\right] - \xi q_y L(\eta_L) \frac{\partial Z_L}{\partial y}$$

$$+ q_{Z_L}\left[1 + \xi L(\eta_L)\right] - q_{Z_o}(1 + \xi) + \xi n \frac{\partial}{\partial t}\left[Z_b + \delta \int_o^{\eta_L} L(\eta)\, d\eta\right]$$
$$= S_o\left[Z_L + \xi\left(Z_b + \delta \int_o^{\eta_L} L(\eta)\, d\eta\right)\right] \frac{\partial s}{\partial t} \tag{4.63}$$

where

$$q_{Z_L} = q_Z \Big|_{Z_L} \tag{4.64}$$

$$q_{Z_o} = q_Z \Big|_{Z_o} \tag{4.65}$$

$L(n_L)$ = value of the influence function at Z_L when $Z_t > Z_L$, otherwise $L(n_L) = 0$

It should be emphasized at this point that the flow equation in the lower zone would have a more complex expression than that of Equation 4.63, if it was rigorously treated analytically. However, considering the inaccuracies inherent in the finite-difference method to be used in solving the problem and the uncertainty related to the parameters describing aquifers' characteristics generally, the approximation of the flow equation for the lower zone seems acceptable.

Equation 4.63 should therefore be the flow equation describing the flow field in the lower zone while Equation 4.62 should describe the flow in the upper zone, the pumpage zone, and in the saltwater zone where the fluid density is constant within each finite-difference block. However, because the flow equations are to be solved simultaneously with the transport equations, a final analysis of the two types of equations will show that the flow equations should be modified.

4.4 Development of the Transport Equations

4.4.1 Transport Equation in the Pumpage Zone

Referring to Figure 4.2, the source of chloride is situated at Z_o. Saline water is not present in the pumpage zone before the top of the transition zone reaches the lower boundary, Z_L, of the pumpage zone. Since the chloride content in the pumpage zone obviously is very small compared to that of the saltwater zone, it is assumed that the concentration gradient in the pumpage zone is negligible; therefore, the

transport in the pumpage zone is purely advective. Furthermore, to reduce the cost of running the model by minimizing the space and computer time, a total mixing (i.e., $\frac{\partial c}{\partial z} = 0$) is assumed in the pumpage zone.

With these assumptions, Equation 4.23 reduces to

$$\nabla \cdot \vec{q}c - \left(\begin{matrix}\text{source}\\ \text{rate}\end{matrix}\right) + \left(\begin{matrix}\text{sink}\\ \text{rate}\end{matrix}\right) = -\frac{\partial nc}{\partial t}$$

which, when expanded and divided by c_s, yields

$$\frac{\partial}{\partial x}\left(q_x \frac{c}{c_s}\right) + \frac{\partial}{\partial y}\left(q_y \frac{c}{c_s}\right) + \frac{\partial}{\partial z}\left(q_z \frac{c}{c_s}\right) - \left(\begin{matrix}\text{source}\\ \text{rates}\end{matrix}\right) + \left(\begin{matrix}\text{sink}\\ \text{rates}\end{matrix}\right) + n\frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) + \frac{c}{c_s}\frac{\partial n}{\partial t} = 0 \qquad (4.67)$$

From Equations 4.52, 4.54 and 4.57, it can be shown that

$$\frac{\partial n}{\partial t} = -S_o \frac{\partial s}{\partial t} \qquad (4.68)$$

and substituting this relationship in 4.67 yields

$$\frac{\partial}{\partial x}\left(q_x \frac{c}{c_s}\right) + \frac{\partial}{\partial y}\left(q_y \frac{c}{c_s}\right) + \frac{\partial}{\partial z}\left(q_z \frac{c}{c_s}\right) - \left(\begin{matrix}\text{source}\\ \text{rates}\end{matrix}\right) + \left(\begin{matrix}\text{sink}\\ \text{rates}\end{matrix}\right) + n\frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) = \left(\frac{c}{c_s}\right) S_o \frac{\partial s}{\partial t} \qquad (4.69)$$

which should therefore be the transport equation in the pumpage zone.

4.4.2 Transport Equations in the Lower Zone

Most of the existing studies of the upconing problem are based on the theory of "sharp interface" which has been suggested by the work of Muskat (1946) and Bear and Dagan (1968). In their work, they assumed for the sake of simplicity that the boundary between the saltwater and the freshwater is an abrupt interface, neglecting thus the effect of the hydrodynamic dispersion. Actually, there exists a transition zone between the two fluids, owing mainly to the hydrodynamic dispersion (Bear and Dagan, 1968; Bear, 1972, 1979; Schmorak and Mercado, 1969). In the

lower zone therefore, both advective and dispersive transports should be considered. The governing equation of the transport phenomena in the lower zone is therefore Equation 4.23.

Dividing both sides of Equation 4.23 by c_s and expanding leads to

$$n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) + \frac{c}{c_s}\frac{\partial n}{\partial t} = \frac{\partial}{\partial x} D_{xx} \frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial x} D_{xy} \frac{\partial}{\partial y}\left(\frac{c}{c_s}\right)$$

$$+ \frac{\partial}{\partial x} D_{xz} \frac{\partial}{\partial z}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial y} D_{yx} \frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial y} D_{yy} \frac{\partial}{\partial y}\left(\frac{c}{c_s}\right)$$

$$+ \frac{\partial}{\partial y} D_{yz} \frac{\partial}{\partial z}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial z} D_{zx} \frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial z} D_{zy} \frac{\partial}{\partial y}\left(\frac{c}{c_s}\right)$$

$$+ \frac{\partial}{\partial z} D_{zz} \frac{\partial}{\partial z}\left(\frac{c}{c_s}\right) - \frac{\partial}{\partial x}\left[q_x \frac{c}{c_s}\right] - \frac{\partial}{\partial y}\left[q_y \frac{c}{c_s}\right]$$

$$- \frac{\partial}{\partial z}\left[q_z \frac{c}{c_s}\right] + \left(\begin{smallmatrix}\text{source}\\ \text{rates}\end{smallmatrix}\right) - \left(\begin{smallmatrix}\text{sink}\\ \text{rates}\end{smallmatrix}\right) \qquad (4.70)$$

With the introduction of Equation 4.68, Equation 4.70 becomes

$$n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) - \left(\frac{c}{c_s}\right) S_o \frac{\partial s}{\partial t} =$$

$$\frac{\partial}{\partial x} D_{xx} \frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial x} D_{xy} \frac{\partial}{\partial y}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial x} D_{xz} \frac{\partial}{\partial z}\left(\frac{c}{c_s}\right)$$

$$+ \frac{\partial}{\partial y} D_{yx} \frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial y} D_{yy} \frac{\partial}{\partial y}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial y} D_{yz} \frac{\partial}{\partial z}\left(\frac{c}{c_s}\right)$$

$$+ \frac{\partial}{\partial z} D_{zx} \frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial z} D_{zy} \frac{\partial}{\partial y}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial z} D_{zz} \frac{\partial}{\partial z}\left(\frac{c}{c_s}\right)$$

$$- \frac{\partial}{\partial x}\left[q_x \frac{c}{c_s}\right] - \frac{\partial}{\partial y}\left[q_y \frac{c}{c_s}\right] - \frac{\partial}{\partial z}\left[q_z \frac{c}{c_s}\right]$$

$$+ \left(\begin{smallmatrix}\text{source}\\ \text{rates}\end{smallmatrix}\right) - \left(\begin{smallmatrix}\text{sink}\\ \text{rates}\end{smallmatrix}\right) \qquad (4.71)$$

Since the relative concentration $\frac{c}{c_s}$ in the lower zone varies from 1 at Z_o to 0 at Z_L, Equation 4.71 should be integrated from Z_o to Z_L in

order to derive the transport equation for the lower zone. Because of the definition of $\frac{c}{c_s}$ within specific limits, the integration should be carried out with respect to those limits. The domains of definition of $\frac{c}{c_s}$ can be summarized as follows:

1. $Z_o < Z < Z_b$

$$\frac{c}{c_s} = 1 \tag{4.72}$$

2. $Z_b < Z < Z_t$

$$\frac{c}{c_s} = L(\eta) \tag{4.73}$$

where

$$\eta = \frac{Z - Z_b}{\delta} \tag{4.74}$$

and for

$$Z = Z_b, \quad \eta = 0 \tag{4.75}$$

$$Z = Z_t, \quad \eta = 1 \tag{4.76}$$

The integration of Equation 4.71 using Leibnitz's rule (Korn and Korn 1961) gives

$$\eta \frac{\partial Z_b}{\partial t} + Z_b\left[\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} - S_o \frac{\partial s}{\partial t}\right] = q_{z_o} - \frac{L'(o)}{\delta}\left[D_{xz} \frac{\partial Z_b}{\partial x} + D_{yz} \frac{\partial Z_b}{\partial y} - D_{zz}\right] \tag{4.77}$$

where

$$q_{z_o} = q_z \Big|_{z_o} \tag{4.78}$$

and

$$n \frac{\partial}{\partial t}\left(\delta \int_0^1 L(\eta)d\eta\right) - \left(\delta \int_0^1 L(\eta)d\eta\right) S_o \frac{\partial s}{\partial t} = \frac{\partial}{\partial x} D_{xx} \frac{\partial}{\partial x}\left(\delta \int_0^1 L(\eta)d\eta\right)$$

$$+ \frac{\partial}{\partial x} D_{xx} \frac{\partial Z_b}{\partial x} + \frac{\partial}{\partial x} D_{xy} \frac{\partial}{\partial y}\left(\delta \int_0^1 L(\eta)d\eta\right) + \frac{\partial}{\partial x} D_{xy} \frac{\partial Z_b}{\partial y}$$

$$- \frac{\partial}{\partial x} D_{xz} + D_{xz} \frac{L'(0)}{\delta} \frac{\partial Z_b}{\partial x} + \frac{\partial}{\partial y} D_{yx} \frac{\partial}{\partial x}\left(\delta \int_0^1 L(\eta)d\eta\right)$$

$$+ \frac{\partial}{\partial y} D_{yx} \frac{\partial Z_b}{\partial x} + \frac{\partial}{\partial y} D_{yy} \frac{\partial}{\partial y}\left(\delta \int_0^1 L(\eta)d\eta\right) + \frac{\partial}{\partial y} D_{yy} \frac{\partial Z_b}{\partial y}$$

$$- \frac{\partial}{\partial y} D_{yz} + D_{yz} \frac{L'(0)}{\delta} \frac{\partial Z_b}{\partial y} - D_{zz} \frac{L'(0)}{\delta}$$

$$- \frac{\partial}{\partial x}\left[q_x \delta \int_0^1 L(\eta)d\eta\right] - q_x \frac{\partial Z_b}{\partial x} - \frac{\partial}{\partial y}\left[q_y \delta \int_0^1 L(\eta)d\eta\right] - q_y \frac{\partial Z_b}{\partial y} \qquad (4.79)$$

where

$$L'(0) = L'(\eta)\Big|_{\eta = 0} \qquad (4.80)$$

and

$$\eta_L = 1 \qquad \text{when } Z_t \leq Z_L \qquad (4.81)$$

$$\eta_L = \frac{Z_L - Z_b}{\delta} \qquad \text{when } Z_t > Z_L \qquad (4.82)$$

Details of the integration are also given in Appendix C.

The integration of Equation 4.71 reveals that the relative concentration $\frac{c}{c_s}$ in the lower zone depends on three parameters: Z_b, the elevation of the saltwater mound; δ, the total thickness of the transition zone; and Z_L, the total thickness of the lower zone.

Even though Equations 4.77 and 4.79 can be solved simultaneously, defining

$$ZDT = Z_b + \delta \int_0^1 L(\eta)\, d\eta \qquad (4.83)$$

and adding Equation 4.77 to 4.79 yields

$$n \frac{\partial}{\partial t}(ZDT) - (ZDT) S_o \frac{\partial s}{\partial t} = \frac{\partial}{\partial x} D_{xx} \frac{\partial}{\partial x}(ZDT) + \frac{\partial}{\partial x} D_{xy} \frac{\partial}{\partial y}(ZDT) - \frac{\partial}{\partial x} D_{xz} + \frac{\partial}{\partial y} D_{yx} \frac{\partial}{\partial x}(ZDT) + \frac{\partial}{\partial y} D_{yy} \frac{\partial}{\partial y}(ZDT) - \frac{\partial}{\partial y} D_{yz} - \frac{\partial}{\partial x}[q_x(ZDT)] - \frac{\partial}{\partial y}[q_y(ZDT)] + q_{z_o} \quad (4.84)$$

The advantage of using Equation 4.84 instead of 4.79 is that the former has only one unknown ZDT, while the latter has two unknowns, Z_b and δ. Once ZDT is known (using 4.84), Equations 4.77 and 4.84 can be used to obtain δ and Z_b.

It should be remembered that Equation 4.84 has been obtained by integrating 4.70 from Z_o to Z_t, while the actual integration should be carried out from Z_o to Z_L. However, since

$$\int_{Z_o}^{Z_L} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz = \int_{Z_o}^{Z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz - \int_{Z_L}^{Z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz \quad (4.85)$$

the use of Equation 4.84 should be completed by the evaluation of $\int_{Z_L}^{Z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz$ which depends on the position of Z_t and Z_b with respect to Z_L.

When $Z_t < Z_L$

$$\int_{Z_L}^{Z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz = 0 \quad (4.86)$$

When $Z_b < Z_L < Z_t$

$$\int_{Z_L}^{Z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz = n \frac{\partial}{\partial t}\left(\delta \int_{n_L}^{1} L(n) dn\right) \quad (4.87)$$

Finally, when $Z_L < Z_b$

$$\int_{Z_L}^{Z_t} n \frac{\partial}{\partial t} \left(\frac{c}{c_s}\right) dz = n \frac{\partial}{\partial t} \left[Z_b + \delta \int_0^1 L(\eta) d\eta\right] = n \frac{\partial}{\partial t} (ZDT) \qquad (4.88)$$

4.5 Reformulation of the Flow and the Transport Equations

The continuity equation (4.1) from which the flow equation (4.59) is derived and the transport equation (4.18) are both mass balance equations. The former is obtained by assuming that the sum of the diffusive and dispersive mass fluxes is negligible compared to the advective one; while this is true for the case analyzed in the pumpage zone, it does not hold in the lower zone. Introducing Equation 4.45 into 4.59 and rearranging terms leads to

$$\frac{\partial}{\partial x} q_x + \frac{\partial}{\partial y} q_y + \frac{\partial}{\partial z} q_z + w(x,y,z,t) - S_o \frac{\partial s}{\partial t}$$

$$+ \frac{1}{\xi} \left[\frac{\partial}{\partial x} \left(\frac{c}{c_s} q_x\right) + \frac{\partial}{\partial y} \left(\frac{c}{c_s} q_y\right) + \frac{\partial}{\partial z} \left(\frac{c}{c_s} q_z\right) + \left(\frac{c}{c_s}\right) w(x,y,z,t)\right.$$

$$\left. + n \frac{\partial}{\partial t} \left(\frac{c}{c_s}\right) - \left(\frac{c}{c_s}\right) S_o \frac{\partial s}{\partial t}\right] = 0 \qquad (4.89)$$

Introducing Equation 4.69 (the transport equation in the pumpage zone) into 4.89 yields

$$\frac{\partial}{\partial x} q_x + \frac{\partial}{\partial y} q_y + \frac{\partial}{\partial z} q_z + w(x,y,z,t) = S_o \frac{\partial s}{\partial t} \qquad (4.90)$$

which is known as the flow equation for constant density fluid flow. However, it is also a "volumetric balance equation" which expresses the property of the incompressibility of the fluid.

What this really suggests is that the flow equation (4.89) is a linear combination of the volumetric balance equation (4.90) and the transport equation (4.69). The comparison of Equations 4.89 and 4.70 shows that the dispersion terms are missing in the flow equation (4.89). Any attempt to solve simultaneously these two equations would lead to erroneous results, unless the dispersion effects are actually neglible. A more general representation of the flow equation would be

$$\frac{\partial}{\partial x} q_x + \frac{\partial}{\partial y} q_y + \frac{\partial}{\partial y} q_z + w(x,y,z,t) - S_o \frac{\partial s}{\partial t}$$

$$+ \frac{1}{\xi} \{ \frac{\partial}{\partial x} (\frac{c}{c_s} q_x) + \frac{\partial}{\partial y} (\frac{c}{c_s} q_y) + \frac{\partial}{\partial z} (\frac{c}{c_s} q_z) + (\frac{c}{c_s}) w(x,y,z,t)$$

$$+ n \frac{\partial}{\partial t} (\frac{c}{c_s}) - (\frac{c}{c_s}) S_o \frac{\partial s}{\partial t} - [\frac{\partial}{\partial x} D_{xx} \frac{\partial}{\partial x} (\frac{c}{c_s}) + \frac{\partial}{\partial x} D_{xy} \frac{\partial}{\partial y} (\frac{c}{c_s})$$

$$+ \frac{\partial}{\partial x} D_{xz} \frac{\partial}{\partial z} (\frac{c}{c_s}) + \frac{\partial}{\partial y} D_{yx} \frac{\partial}{\partial x} (\frac{c}{c_s}) + \frac{\partial}{\partial y} D_{yy} \frac{\partial}{\partial y} (\frac{c}{c_s}) + \frac{\partial}{\partial y} D_{yz} \frac{\partial}{\partial z} (\frac{c}{c_s})$$

$$+ \frac{\partial}{\partial z} D_{zx} \frac{\partial}{\partial x} (\frac{c}{c_s}) + \frac{\partial}{\partial z} \partial_{zy} \frac{\partial}{\partial y} (\frac{c}{c_s}) + \frac{\partial}{\partial z} D_{zz} \frac{\partial}{\partial z} (\frac{c}{c_s})]\} = 0 \qquad (4.91)$$

However, using the assumption of non-compressible fluids, the three-dimensional flow equation for the aquifer system is simply

$$\frac{\partial}{\partial x} q_x + \frac{\partial}{\partial y} q + \frac{\partial}{\partial z} q_z + w(x,y,z,t) = S_o \frac{\partial s}{\partial t} \qquad (4.92)$$

(previously obtained as Equation 4.90).

The transport equation (4.71) for the lower zone is obtained by integrating Equation 4.70 from Z_o (the lower boundary of the lower zone) to Z_t the top of the transition zone. This approach which simplifies the computation of δ and Z_b, parameters which define $\frac{c}{c_s}$ in the lower zone, hides however the details on the vertical component of the solute leaving the lower zone and going into the pumpage zone. The global vertical component of 4.70 leaving the lower zone and going into the pumpage zone is however known as

$$n \int_{Z_L}^{Z_t} \frac{\partial}{\partial t} \left(\frac{c}{c_s}\right) dz,$$

after the transition zone reaches the pumpage zone. This term accounts for both the advective and the dispersive terms. In the pumpage zone however, because of the assumption of no dispersion, the vertical component of the solute coming from the lower zone is only the advective term $\frac{1}{\beta p}\left(\frac{c}{c_s}\right)q_{z_L}$ [from the term $\frac{\partial}{\partial x}\left(\frac{c}{c_s}q_z\right)$]; in order for the model to be consistent, the term $\left(\frac{c}{c_s}\right)q_{z_L}$ in the pumpage zone transport equation will be replaced by $n\int_{Z_L}^{Z_t}\frac{\partial}{\partial t}\left(\frac{c}{c_s}\right)dz$. It should be remembered that the method of solution in the present study is the finite-difference method; all the approximations being made here are consistent with that method. For example,

$$\frac{\partial}{\partial z}\left(\frac{c}{c_s} q_z\right) = \frac{\frac{c}{c_s} q_{z\,z_p} - \frac{c}{c_s} q_{z\,z_L}}{Z_L - Z_p} \qquad (4.93)$$

and since $\frac{c}{c_s}$ in the upper zone is zero, Equation 4.93 becomes

$$\frac{\partial}{\partial z}\left(\frac{c}{c_s} q_z\right) = - \frac{\left.\frac{c}{c_s} q_z\right|_{z_L}}{BP} \tag{4.94}$$

where

$$BP = z_p - z_L$$

z_p being the elevation of the top of the pumpage zone. Replacing $\left.\frac{c}{c_s} q_z\right|_{z_L}$ by $n\int_{z_L}^{z_t} \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz$ in Equation 4.94 gives

$$\frac{\partial}{\partial z}\left(\frac{c}{c_s} q_z\right) = - \frac{n\int_{z_L}^{z_t} \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz}{BP} \tag{4.95}$$

On the other hand, Equations 4.77 and 4.84 should be equivalent when the effect of the mechanical dispersion is neglected (i.e., $a_L = a_T = 0$), since the latter is the cause of the development of the transition zone. Hence, for $a_L = a_T = 0$, the dispersion coefficients vanish and Equations 4.77 and 4.84 become, respectively

$$n \frac{\partial Z_b}{\partial t} - Z_b \left(S_o \frac{\partial s}{\partial t}\right) = - Z_b \frac{\partial q_x}{\partial x} - Z_b \frac{\partial q_y}{\partial y} + q_{z_o} \tag{4.96}$$

and

$$n \frac{\partial Z_b}{\partial t} - Z_b \left(S_o \frac{\partial s}{\partial t}\right) = - \frac{\partial}{\partial x}\left[q_x Z_b\right] - \frac{\partial}{\partial y}\left[q_y Z_b\right] + q_{z_o} \tag{4.97}$$

The subtraction of Equation 4.96 from 4.97 leads to

$$- q_x \frac{\partial Z_b}{\partial x} - q_y \frac{\partial Z_b}{\partial y} = 0 \tag{4.98}$$

In order for Equations 4.96 and 4.97 to be equivalent, 4.98 should be verified. However, the combination of Equation 4.98 with 4.77 yields

$$n \frac{\partial Z_b}{\partial t} - Z_b \left(S_o \frac{\partial s}{\partial t}\right) = - \frac{\partial}{\partial x}\left(q_x Z_b\right) - \frac{\partial}{\partial y}\left(q_y Z_b\right) + q_{z_o} - \frac{L'(o)}{\delta}\left[D_{xz} \frac{\partial Z_b}{\partial x} + D_{yz} \frac{\partial Z_b}{\partial y} - D_{zz}\right] \quad (4.99)$$

and, by using 4.99 as the equation describing the movement of the saltwater front Z_b, ZDT becomes equivalent to Z_b when the dispersion coefficients vanish. The transport equation in the lower zone is finally represented by Equations 4.84 and 4.99. Equation 4.83 will still be used to determine the thickness of the transition zone δ.

4.6 Initial and Boundary Conditions

The differential equations presented in the previous paragraphs have an infinite number of solutions; in order for a mathematical model to represent a specific physical problem, additional information must be provided along with the governing differential equations. This complementary information includes the geometry of the physical system as presented in Section 4.1, e.g., values of all physical coefficients, such as the hydraulic conductivity tensor, and the dispersion tensor. Those usually are obtained through the analysis of experimental or field data and the initial and boundary conditions.

4.6.1 Initial Conditions

Initial conditions are the specification of all relevant dependent variables of the governing equations at all points within the domain of definition of the aquifer system, at some initial time usually denoted t_o. In the present analysis the initial conditions are

$$s = s_o(x,y,z,o) \tag{4.100}$$

$$\frac{\rho}{\rho_f} = \frac{\rho_o}{\rho_f}(x,y,z,o) \tag{4.101}$$

and

$$\frac{c}{c_s} = \frac{c_o}{c_s}(x,y,o) \tag{4.102}$$

$$\delta = \delta_o(x,y,o) \tag{4.103}$$

$$Z_b = Z_b(x,y,o) \tag{4.104}$$

where

$s_o(x,y,z,o)$ is the distribution of the drawdown throughout the flowfield at time t_o;

$\frac{\rho_o}{\rho_f}(x,y,z,o)$ is the distribution of the relative density throughout the flow field at time t_o;

$\frac{c_o}{c_s}(x,y,o)$ is the distribution of the relative concentration in the pumpage zone at time t_o;

$\delta_o(x,y,o)$ and $Z_{bo}(x,y,o)$ are, respectively, the distribution of the thickness of the transition zone and the distribution of the rise of the saltwater mound in the lower zone at time t_o.

4.6.2 Boundary Conditions

In the theory of partial differential equations applied to subsurface hydrology, there exist three types of boundary conditions: first, boundary of prescribed potential; second, boundary of prescribed flux; and third, mixed boundary condition.

(a) Boundary of prescribed potential.

In this boundary condition, known as Dirichlet or first type boundary condition, the potential ϕ is prescribed for all points of the boundary. Mathematically, it is expressed

$$\phi = F(x,y,z,t) \tag{4.105}$$

on the boundary; from the transformation of the dependent variable used in the present study, Equation 4.105 becomes

$$s = G(x,y,z,t) \tag{4.106}$$

F and G are known functions.

In the application of finite-difference methods to groundwater flow problems associated with pumping wells, the governing differential equations are applied to a finite domain bounded in the horizontal (x,y) plane by a boundary, usually a rectangle. That boundary customarily has the Dirichlet boundary condition when the rectangle is large enough, so that the pumpage does not affect the potential at the boundary. Physical boundaries such as lakes and rivers can change the horizontal shape of the boundary.

In the present work, the boundary of the aquifer in the x,y plane is considered a rectangle large enough to consider the drawdowns distribution at the boundary constant. Hence, Equation 4.106 applies.

(b) Boundary of prescribed flux.

On the boundary of this type, the flux normal to the boundary surface is prescribed for all points of the boundary. Mathematically, it is stated as $q_n = Q(x,y,z,t)$ where Q is a known function. This type of boundary condition is called second type or Neuman boundary condition.

The confining layer at the bottom of the saltwater zone has a second type boundary condition since q_z is zero at that boundary.

(c) Mixed boundary condition.

This type of boundary condition known as third type or Cauchy boundary is defined by specifying the head ϕ in an adjacent aquifer and allowing a flow through a semipervious layer in or out of the considered aquifer. Mathematically, it is expressed as

$$q_n = K' \frac{\phi_a - \phi}{B'} \tag{4.107}$$

and in the present work

$$q_n = K' \frac{s - s_a}{B'} \tag{4.108}$$

where ϕ_a and s_a are, respectively, the piezometric head and the drawdown in the adjacent aquifer, ϕ and s are the piezometric head and the drawdown in the main aquifer; K' and B' are, respectively, the hydraulic conductivity and the thickness of the semipermeable layer. The ratio B'/K' is defined as the resistance of the semipermeable layer (Bear, 1979).

In the present work, the boundary on top of the upper layer is a boundary condition of the third kind.

(d) Boundary condition of the solute transport equation.

The boundary of the aquifer domain, in the horizontal plane, is a rectangle large enough so that $\frac{c}{c_s}$ in the pumpage zone, δ and Z_b in the lower zone are constant at the boundary. The value of $\frac{c}{c_s}$ is equal to 1 and remains constant at Z_o, the boundary between the lower zone and the saltwater zone, while it is zero in the upper zone and in the water table.

CHAPTER 5
NUMERICAL FORMULATION OF THE UPCONING PROBLEM

5.1 Finite-Difference Methods

Over the last two decades, the use of mathematical models has gained wide acceptance throughout the field of underground hydrology. A mathematical model of a physical system is a set of partial differential equations, together with an appropriate set of boundary conditions, which is believed to adequately describe the significant physical process or processes taking place in the physical system (Peaceman, 1977).

Most underground flow problems are so complex that their solution by means of analytical methods requires extensive simplifying assumptions which are sometimes unrealistic. The interest in the development of numerical methods applied to subsurface flow problems derives from the need of solving very complex groundwater flow problems without resorting to simplifications that transform the physical system into an unrealistic one. The finite-difference technique is probably the oldest of the numerical techniques used in solving the mathematical model of very complex physical systems (Remson et al. 1971).

A numerical procedure for solving a transient groundwater problem (or parabolic equations generally), consists of some stepwise methods for obtaining the solution of the problem at time level t_{k+1} from a solution already known at time level t_k. Thus, proceeding from an initial condition (at $t = t_0$), the solution at time t_1 ($t_1 = t_0 + \Delta t_1$)

is obtained; using the solution at time t_1 as the new initial condition, the solution at time t_2 ($t_2 = t_1 + \Delta t_2$) is obtained. Hence, the solution "marches" through time.

The purpose of this chapter is not to discuss the finite-difference methods. The finite-difference methods for solving partial differential equations have been the subject of many books; details of the techniques and most of their applications as well as detailed bibliography of the topic can be seen in Remson et al. (1971), Ames (1977), and Peaceman (1977). Suffice it to say that the basic idea of finite-difference methods is to replace derivatives at a point by ratios of the changes in appropriate variables over a small but finite interval. For example,

$$\frac{\partial \phi}{\partial t} \approx \frac{\Delta \phi}{\Delta t} \tag{5.1a}$$

$$\frac{\partial \phi}{\partial x} \approx \frac{\Delta \phi}{\Delta x} \tag{5.1b}$$

The finite-difference analogs to partial differential equations are of two types: explicit analogs and implicit analogs.

An explicit analog is the expression of an unknown variable, generally at time step k + 1 in terms of known variables, generally at time step k. An example of an explicit analog is

$$\phi_i^{k+1} = a_0 + a_1\phi_1^k + \cdots + a_j\phi_j^k + \cdots + a_N\phi_N^k \tag{5.2}$$

$i = 1,N$

Explicit analogs generally are subject to problems known in the finite-difference literature as stability and convergence problems.

A finite-difference method is said to be convergent if the derived numerical solution approaches the analytical solution when the finite intervals approach zero (i.e., $\frac{\Delta \phi}{\Delta t} \to \frac{\partial \phi}{\partial t}$ when $\Delta \phi$, $\Delta t \to 0$; Remson et al.,

1971). On the other hand, a finite-difference method is said to be stable when the effect of an error made in one stage of the computation is not amplified in later stages of the computation (Peaceman, 1977). Generally, however, convergence and stability are functions of the same variables, usually stated as a relationship of the time increment Δt to the space variable intervals Δx (and/or Δy and Δz). The general form of the most common stability-convergence criteria for models similar to the current one are as follows:

$$\alpha \frac{\Delta t}{\Delta x} < C_1 \tag{5.3}$$

or

$$\beta \frac{\Delta t}{(\Delta x)^2} < C_2 \tag{5.4}$$

where C_1 and C_2 are real constant numbers while α and β are combinations of some physical characteristics of the physical system (e.g., $\beta = \frac{T}{S}$ for a two-dimensional underground transient flow simulation with T = transmissivity of the aquifer and S = storage coefficient).

Implicit methods generally express an unknown variable in terms of known and unknown variables, hence transforming the partial differential equation into a set of simultaneous difference equations which are simple to solve in cases where only one space variable is involved. However, their solutions on a high speed computer become very complex when more than one space variable is concerned. They converge generally and are usually stable, allowing therefore the use of larger time increments and decreasing the number of steps to a final solution at time t_n. There is therefore a need to find an efficient, accurate means of formulating the problem for solution by implicit techniques.

In 1955, Peaceman and Rachford proposed the "Alternating-Direction-Implicit" (ADI) method for the solution of transient flow problems with

two space variables. The method was then extended to three space variables by Douglas and Rachford (1956), by Brian (1961) and by Douglas (1962).

Even though the ADI methods seem to lack a well-defined theory, several applications so far have proved their capability, when adequately used, of solving very complex problems while preserving unconditional stability and reasonable accuracy (Remson et al., 1971; Peaceman 1977; and Prickett and Lonnquist, 1971). In the present work, the ADI method suggested by Brian (1961) and Douglas (1962) has been adapted to the solution of the upconing problem.

5.2 Finite-Difference Grid System

Two types of grid systems are generally considered in finite-difference methods: block centered grid and point centered grid. Despite the semantic difference, the two types of grid systems are closely related; Peaceman (1977) gives some general ideas about what distinguishes one from the other. The block-centered grid, used in the present work can be defined as follows.

Considering the conceptual representation of the aquifer shown on Figure 5.1 as a block of size X_1, Y_1, and Z_1, this block can be subdivided into N•M•K small blocks (Figure 5.2) by dividing X_1 by N intervals, Y_1 by M intervals and Z_1 by K intervals.

The point $P(x_i, y_j, z_k)$ at the center of the block (i,j,k) will simply be defined by $P_{i,j,k}$ and be representative of the block (i,j,k). When the subscript k is well defined as, say, Lower zone, then, variables at $P_{i,j,k}$ will bear only the subscript i,j (i.e., $sL_{i,j}$ instead of $s_{i,j,k}$).

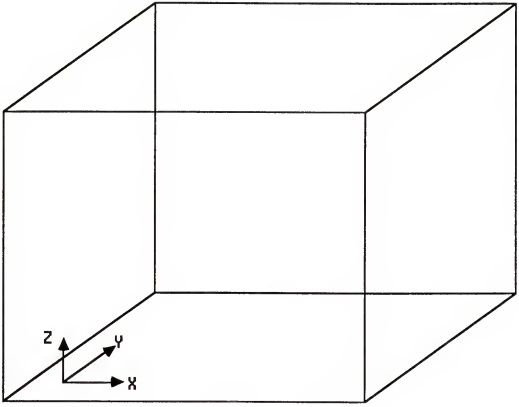


Figure 5.1 Representation of the Aquifer as a Single Block

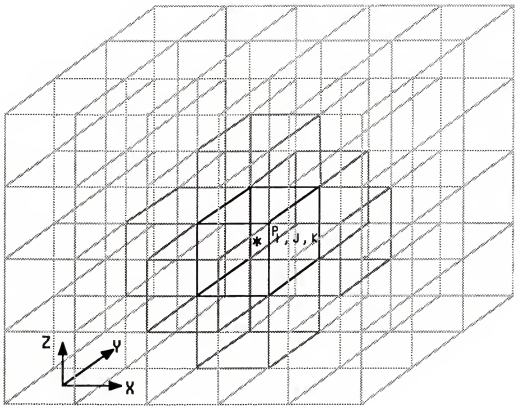


Figure 5.2 Finite Difference Discretization of the Aquifer System

5.3 Finite-Difference Analogs of the Derivatives in the Flow and the Transport Equations

5.3.1 First Derivative Approximations

The elementary finite-difference approximations are discussed in Remson et al. (1971), Ames (1977), and Peaceman (1977). The commonly used approximations of a first derivative are as follows:

(a) Backward difference,

$$\left(\frac{\partial s}{\partial x}\right)_{i,j,k} = \frac{s_{i,j,k} - s_{i-1,jk}}{\Delta x} \tag{5.5}$$

(b) Forward difference,

$$\left(\frac{\partial s}{\partial x}\right)_{i,j,k} = \frac{s_{i+1,j,k} - s_{i,j,k}}{\Delta x} \tag{5.6}$$

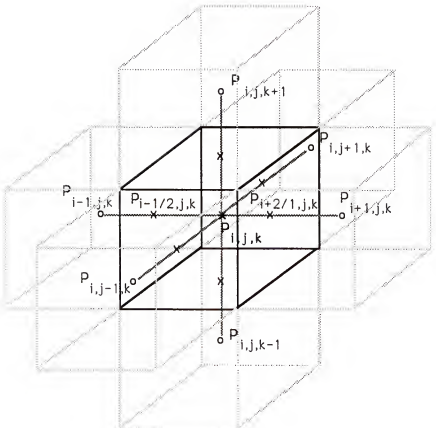
(c) Central difference,

$$\left(\frac{\partial s}{\partial x}\right)_{i,j,k} = \frac{s_{i+1,j,k} - s_{i-1,j,k}}{2\Delta x} \tag{5.7}$$

A variant of Equation 5.7 is

$$\left(\frac{\partial q_x}{\partial x}\right)_{i,j,k} = \frac{q_{x_{i+\frac{1}{2},j,k}} - q_{x_{i-\frac{1}{2},j,k}}}{\Delta x} \tag{5.8}$$

In Equation 5.8, $q_{x_{i+\frac{1}{2},j,k}}$ represents the specific discharge at the midpoint $P_{i+\frac{1}{2},j,k}$ situated at a distance $\frac{\Delta x}{2}$ from each of the end-points $P_{i,j,k}$ and $P_{i+1,j,k}$ (Figure 5.3). Similarly, $q_{x_{i-\frac{1}{2},j,k}}$ represents the specific discharge at the mid-point $P_{i-\frac{1}{2},j,k}$ between $P_{i-1,j,k}$ and $P_{i,j,k}$. Hereafter, unless otherwise specified, this notation will be used without further explanation to express mid-point values in x, y, and z directions and also to express half-time value (e.g., $s^{n+\frac{1}{2}}_{i,j,k}$ is the value of the drawdown at $P_{i,j,k}$, at time $t_n + \frac{\Delta t}{2}$).



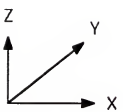


Figure 5.3 Representation of the Nodal and Middle Points.

In the finite-difference theory, assuming a linear variation of a variable, the following expressions

$$q_{x_{i+1/2,j,k}} = \frac{1}{2}\left(q_{x_{i,j,k}} + q_{x_{i+1,j,k}}\right) \tag{5.9}$$

$$q_{x_{i-1/2,j,k}} = \frac{1}{2}\left(q_{x_{i,j,k}} + q_{x_{i-1,j,k}}\right) \tag{5.10}$$

are commonly used to express the mid-point values when the end-point values are known. In a similar way, when the mid-point values are known, the following expression,

$$q_{x_{i,j,k}} = \frac{1}{2}\left(q_{x_{i+1/2,j,k}} + q_{x_{i-1/2,j,k}}\right) \tag{5.11}$$

can be used to estimate the node point value $q_{x_{i,j,k}}$.

The finite-difference approximations are generally expressed with an error term which sometimes is used to estimate how good the approximation is. Nevertheless, the preference of any approximation depends on the type of problem being analyzed (Peaceman 1977). It should also be said that there exist many other ways of approximating a first derivative. In the present work, however, Expression 5.8 is preferred to the others, specifically for the computation of the Darcy's velocity distribution. The following discussion explains the reasons for this preference.

The mean specific discharge in the x direction $\bar{q}_{x_{i+(i+1),j,k}}$ between two end-points $P_{i+1,j,k}$ and $P_{i,j,k}$ can be expressed as

$$\bar{q}_{x_{i+(i+1),j,k}} = \frac{1}{x_{i+1} - x_i}\int_{x_i}^{x_{i+1}} q_x dx \tag{5.12}$$

Introducing Equation 4.58 into 5.12 leads to

$$q_{x_{i\div(i+1),j,k}} = \frac{1}{x_{i+1} - x_i} \int_{x_i}^{x_{i+1}} K_{x_{j,k}} \frac{\partial s}{\partial x} \, dx \tag{5.13}$$

and assuming that the hydraulic conductivity $K_{x_{j,k}}$ is constant between the considered points, the expression of the mean specific discharge in x direction between $P_{i,j,k}$ and $P_{i+1,j,k}$ takes the form

$$\overline{q}_{x_{i\div(i+1),j,k}} = K_{x_{j,k}} \frac{s_{i+1,j,k} - s_{i,j,k}}{x_{i+1} - x_i} \tag{5.14}$$

Defining

$$\Delta x = x_{i+1} - x_i$$

$$\Delta s = -\Delta\phi = s_{i+1,j,k} - s_{i,j,k}$$

Expression 5.14 becomes

$$\overline{q}_{x_{i\div(i+1),j,k}} = K_{x_{j,k}} \frac{s_{i+1,j,k} - s_{i,j,k}}{\Delta x} \tag{5.15}$$

or

$$\overline{q}_{x_{i\div(i+1),j,k}} = -K_{x_{j,k}} \left(\frac{\Delta\phi}{\Delta x}\right) \tag{5.16}$$

Application of 5.8 at $P_{i+1/2,j,k}$ gives

$$\left(\frac{\partial s}{\partial x}\right)_{i+1/2,j,k} = \frac{s_{i+1,j,k} - s_{i,j,k}}{\Delta x} \tag{5.17}$$

which, introduced into Equation 5.15, leads to

$$\overline{q}_{x_{i\div(i+1),j,k}} = K_{x_{j,k}} \left(\frac{\partial s}{\partial x}\right)_{i+1/2,j,k} \tag{5.18}$$

which suggests that the local value of the derivative $\frac{\partial s}{\partial x}$ at $x_i + \frac{\Delta x}{2}$ is the same as the average value of $\frac{\partial s}{\partial x}$ between x_i and x_{i+1}, with the assumption of constant hydraulic conductivity $K_{x_{j,k}}$ between x_i and

x_{i+1}. In order for that approximation to be physically accurate, points $P_{i,j,k}$ and $P_{i+1,j,k}$ should evidently be very close, unless the problem concerns a special type of flow field (e.g., one-dimensional uniform flow). This explains, in part, the condition of convergence in the finite-difference theory. Another inference of Equation 5.17 is that the backward difference gives the exact average-value of the derivative between points $P_{i-1,j,k}$ and $P_{i,j,k}$; the forward difference gives the exact average-value of the derivative between points $P_{i,j,k}$ and $P_{i+1,j,k}$; the central difference expressed by Equation 5.7 gives the exact average value between points $P_{i-1,j,k}$ and $P_{i+1,j,k}$ while the one expressed by Equation 5.8 gives the exact average value between mid-points $P_{i-\frac{1}{2},j,k}$ and $P_{i+\frac{1}{2},j,k}$. Since the condition for a local value at mid-point to be approximated by the average value between the two end-points is that those two end-points be as close as possible, Equation 5.8 evidently expresses the best approximation of the first derivative at $P_{i,j,k}$.

In the analysis of groundwater flow problems, a well is generally considered as a singularity. One of the characteristics of well hydraulics is the change of flow direction at the well (i.e., $q_{x_{(i-1)\mp i,j,k}}$ and $q_{x_{i\mp(i+1),j,k}}$ are of opposite directions if the well is at the node $P_{i,j,k}$), with a net zero horizontal velocity at the well itself. The use of central differences in the form of Equation 5.7 for the computation of nodal Darcy-velocities becomes very delicate. On the other hand, the transport process is more concerned with velocity between pairs of points than that at the points themselves; and, the drawdowns at nodal points are more desirable than the drawdowns between pairs of points. Therefore, in what follows, specific discharges between pairs

of points will be considered and will be estimated by Equation 5.15 (average specific discharge between pairs of points, assumed to be the value of the specific discharge at the mid-points of the pairs of points). The nodal specific discharges, when needed, will be computed using Equation 5.11.

Finally, Equation 5.16, which is equivalent to Expression 5.15, is very similar to the original formula which Darcy (1856) obtained from his experimental study.

Special attention should be paid to the approximation of some types of first derivatives in the flow and transport equations (Equation 4.69, 4.77, 4.79, 4.84, 4.92, and 4.95). For instance application of Equation 5.8 to terms of the form $\frac{\partial}{\partial x}[q_x(ZDT)]$ gives:

$$\frac{\partial}{\partial x}[q_x(ZDT)]_{i,j} = \frac{1}{\Delta x}\{q_{x_{i+1/2,j}}(ZDT)_{i+1/2,j} - q_{x_{i-1/2,j}}(ZDT)_{i-1/2,j}\} \tag{5.19}$$

and replacing $(ZDT)_{i+1/2,j}$ and $(ZDT)_{i-1/2,j}$ by their equivalent expressions (Equations 5.9 and 5.10) in terms of $(ZDT)_{i-1,j}$, $(ZDT)_{i,j}$, $(ZDT)_{i+1,j}$; and rearranging the terms, leads to

$$\frac{\partial}{\partial x}[q_x(ZDT)]_{i,j} = \frac{.5}{\Delta x}\{q_{x_{i+1/2,j}}(ZDT)_{i+1,j} + [q_{x_{i+1/2,j}} - q_{x_{i-1/2,j}}](ZDT)_{i,j} - q_{x_{i-1/2,j}}(ZDT)_{i-1,j}\} \tag{5.20}$$

It should be noticed that the approximation of $\frac{\partial}{\partial x}(q_x \frac{c}{c_s})$ has the same form as Equation 5.20. While this approximation apparently does not seem to pose a major problem in the computation of the ZDT's, for large values of Δt (20 days for instance), it gives negative

concentrations at the points surrounding the well in the pumpage zone. A possible explanation of that behavior is as follows: the first point in the pumpage zone to be reached by the transition zone is the "well node" (the node at which the well is; at that time, the solute concentration at the points surrounding the well (Figure 5.4) is zero, i.e., $(\frac{c}{c_s})_{i-1,j} = (\frac{c}{c_s})_{i+1,j} = (\frac{c}{c_s})_{i,j+1} - 0)$, while the specific discharges are toward the well. Rewriting 5.19 (in terms of $\frac{c}{c_s}$) as

$$\frac{\partial}{\partial x}\left(q_x \frac{c}{c_s}\right)_{i,j} = \frac{1}{\Delta x}\left\{q_{x_{i+1/2,j}} \frac{\left[\left(\frac{c}{c_s}\right)_{i+1,j} + \left(\frac{c}{c_s}\right)_{i,j}\right]}{2} - q_{x_{i-1/2,j}} \frac{\left[\left(\frac{c}{c_s}\right)_{i,j} + \left(\frac{c}{c_s}\right)_{i-1,j}\right]}{2}\right\} \tag{5.21}$$

and for $(\frac{c}{c_s})_{i-1,j} = (\frac{c}{c_s})_{i+1,j} = 0$, from 5.21

$$\frac{\partial}{\partial x}\left(q_x \frac{c}{c_s}\right)_{i,j} = \frac{1}{2\Delta x}\left[q_{x_{i+1/2,j}} - q_{x_{i-1/2,j}}\right]\left(\frac{c}{c_s}\right)_{i,j} \tag{5.22}$$

Since $q_{x_{i+1/2}}$ and $q_{x_{i-1/2,j}}$ are non-zero and of opposite direction, and since $(\frac{c}{c_s})_{i,j}$ is also non-zero, Expression 5.22 is different from zero. Actually,

$$\frac{\partial}{\partial x}\left(q_x \frac{c}{c_s}\right) = \text{(flux-IN-flux-OUT) in x direction} \tag{5.23}$$

and from Figure 5.4, it is obvious that $\frac{\partial}{\partial x}(q_x \frac{c}{c_s})$ is zero. This causes what in the literature of finite-difference method is termed "numerical dispersion," and has different explanations depending on the mathematical approach used to explain it. Several methods are suggested to minimize the effect of the numerical dispersion (Peaceman, 1977; Ames,

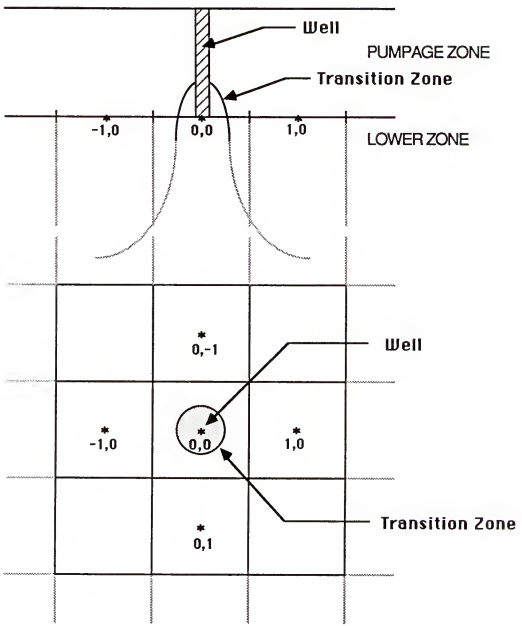


Figure 5.4 Cross and Plan View of the Transition Zone Reaching the Well Node Only, in the Pumpage Zone

1977; Remson et al., 1971). However, none of those methods can actually eliminate the effect of the numerical dispersion completely. The approach used in the present study is the development of an algorithm which checks the direction of the flow around the nodal point and uses the following approximation

$$\frac{\partial}{\partial x}\left(q_x \frac{c}{c_s}\right)_{i,j} = \frac{1}{\Delta x}\left(q_{x_{i+1/2,j}} \begin{Bmatrix} (+)\ (\frac{c}{c_s})_{i,j} \\ (-)\ (\frac{c}{c_s})_{i+1,j} \end{Bmatrix} - q_{x_{i-1/2,j}} \begin{Bmatrix} (+)\ (\frac{c}{c_s})_{i-1,j} \\ (-)\ (\frac{c}{c_s})_{i,j} \end{Bmatrix}\right) \tag{5.24}$$

The signs in parentheses indicate the direction of the specific discharges $q_{x_{i+1/2,j}}$ and $q_{x_{i-1/2,j}}$; the term following the sign is used instead of half of the sum of the term in the brackets, as in Equation 5.21. Referring to Figure 5.4, application of 5.24 to the well node gives

$$\frac{\partial}{\partial x}\left(q_x \frac{c}{c_s}\right)_{i,j} = \frac{1}{\Delta x}\left[q_{x_{i+1/2,j}} (\frac{c}{c_s})_{i+1,j} - q_{x_{i-1/2,j}} (\frac{c}{c_s})_{i-1,j}\right] \tag{5.25}$$

because $q_{x_{i+1/2,j}}$ is negative while $q_{x_{i-1/2,j}}$ is positive. Hence, for $(\frac{c}{c_s})_{i-1,j} = (\frac{c}{c_s})_{i+1,j} = 0$, Equation 5.25 reduces to

$$\frac{\partial}{\partial x}\left(q_x \frac{c}{c_s}\right)_{i,j} = 0 \tag{5.26}$$

which is the exact value sought. Applying 5.21 to the node (i-1,j) gives

$$\frac{\partial}{\partial x}\left(q_x \frac{c}{c_s}\right)_{i-1,j} = \frac{1}{\Delta x}\left\{q_{x_{i-1/2,j}} \frac{\left[(\frac{c}{c_s})_{i,j} + (\frac{c}{c_s})_{i-1,j}\right]}{2} - q_{x_{i-3/2,j}} \frac{\left[(\frac{c}{c_s})_{i-2,j} + (\frac{c}{c_s})_{i-1,j}\right]}{2}\right\} \tag{5.27}$$

which for $(\frac{c}{c_s})_{i-1,j} = (\frac{c}{c_s})_{i-2,j} = 0$, yields

$$\frac{\partial}{\partial x}(q_x \frac{c}{c_s})_{i-1,j} = \frac{1}{2\Delta x} q_{x_{i-1/2,j}} (\frac{c}{c_s})_{i,j} \tag{5.28}$$

while the application of 5.24 gives

$$\frac{\partial}{\partial x}(q_x \frac{c}{c_s}) = \frac{1}{\Delta x} \{q_{x_{i-1/2,j}} (\frac{c}{c_s})_{i-1,j} - q_{x_{i-3/2,j}} (\frac{c}{c_s})_{i-2,j}\} = 0 \tag{5.29}$$

The algorithm 5.24 is therefore the method used to handle the advective terms of the form $\frac{\partial}{\partial x}[q_x(\frac{c}{c_s})]$ in the transport equations.

On the other hand, a straightforward application of Equation 5.7 to expression of the form $q_x \frac{\partial Z_b}{\partial x}$ leads to:

$$q_x \frac{\partial Z_b}{\partial x}_{i,j} = q_{x_{i,j}} \frac{Z_{b_{i+1,j}} - Z_{b_{i-1,j}}}{2\Delta x} \tag{5.30}$$

However, knowing that

$$q_x \frac{\partial Z_b}{\partial x} = \frac{\partial}{\partial x}(q_x Z_b) - Z_b \frac{\partial q_x}{\partial x} \tag{5.31}$$

writing

$$Z_b \frac{\partial q_x}{\partial x}_{i,j} = Z_{b_{i,j}} \frac{q_{x_{i+1/2,j}} - q_{x_{i-1/2,j}}}{\Delta x} \tag{5.32}$$

and, by analogy to Equation 5.20

$$\frac{\partial}{\partial x}(q_x Z_b) = \frac{.5}{\Delta x} \{q_{x_{i+1/2,j}} Z_{b_{i+1,j}} + [q_{x_{i+1/2,j}} - q_{x_{i-1/2,j}}] Z_{b_{i,j}} - q_{x_{i-1/2,j}} Z_{b_{i-1,j}}\} \tag{5.33}$$

subtracting Equation 5.23 from 5.24 gives

$$q_x \frac{\partial Z_b}{\partial x}_{i,j} = \frac{+5}{\Delta x} \{ q_{x_{i+\frac{1}{2},j}} Z_{b_{i+1,j}} - [q_{x_{i+\frac{1}{2},j}} - q_{x_{i-\frac{1}{2},j}}] Z_{b_{i,j}} - q_{x_{i-\frac{1}{2},j}} Z_{b_{i-1,j}} \} \quad (5.34)$$

The main difference between Equations 5.30 and 5.34 is that the former assumes $q_{x_{i,j}}$ to be the mean specific discharge in x direction between points $P_{i-1,j}$ and $P_{i+1,j}$ while the latter considers the average values of the specific discharge between pairs of points (i.e., $q_{x_{i-\frac{1}{2},j}}$ between $P_{i-1,j}$ and $P_{i,j}$; $q_{x_{i+\frac{1}{2},j}}$ between $P_{i,j}$ and $P_{i+1,j}$).

Equation 5.34 can also be obtained using 5.11 and writing

$$(q_x \frac{\partial Z_b}{\partial x})_{i,j} = \frac{1}{2} [(q_x \frac{\partial Z_b}{\partial x})_{i+\frac{1}{2},j} + (q_x \frac{\partial Z_b}{\partial x})_{i-\frac{1}{2},j}]$$

$$= \frac{1}{2} [q_{x_{i+\frac{1}{2},j}} \frac{(Z_{b_{i+1,j}} - Z_{b_{i,j}})}{\Delta x} - q_{x_{i-\frac{1}{2},j}} \frac{(Z_{b_{i,j}} - Z_{b_{i-1,j}})}{\Delta x}]$$

$$= \frac{+5}{\Delta x} \{ q_{x_{i+\frac{1}{2},j}} Z_{b_{i+1,j}} - [q_{x_{i+\frac{1}{2},j}} - q_{x_{i-\frac{1}{2},j}}] Z_{b_{i,j}} - q_{x_{i-\frac{1}{2},j}} Z_{b_{i-1,j}} \}$$

The purpose of the approach used in deriving 5.34 is to show its relationship with 5.33 of which the inaccuracy is already discussed. Nevertheless, the transformation of Equation 4.79 into 4.84 reduces the use of 5.34 to the approximation of terms like $D_{xy} \frac{\partial Z_b}{\partial x}$ and $D_{yx} \frac{\partial Z_b}{\partial y}$ (in Equation 4.77) and the present study considers that the errors introduced by those approximations are acceptable.

The flow equations are solved before the transport equations; therefore, Equation 5.34 is well defined (i.e., the q's in Equation 5.34

are defined by the drawdowns obtained using the flow equation, 5.50) for the computation of the rise of the saltwater mound Z_b.

5.3.2 Second Derivative Approximations

Numerous second derivative terms appear in the equations. The approximation of these second derivatives is obtained in the following way:

by analogy to Equation 5.8,

$$\frac{\partial}{\partial x}\left[D_{xx}\frac{\partial(ZDT)}{\partial x}\right]_{i,j} = \frac{1}{\Delta x}\left\{D_{xx_{i+\frac{1}{2},j}}\left[\frac{\partial(ZDT)}{\partial x}\right]_{i+\frac{1}{2},j} - D_{xx_{i-\frac{1}{2},j}}\left[\frac{\partial(ZDT)}{\partial x}\right]_{i-\frac{1}{2},j}\right\} \quad (5.35)$$

where, also by analogy to Equation 5.8,

$$\left(\frac{\partial(ZDT)}{\partial x}\right)_{i+\frac{1}{2},j} = \frac{(ZDT)_{i+1,j} - (ZDT)_{i,j}}{\Delta x} \quad (5.36a)$$

and

$$\left(\frac{\partial(ZDT)}{\partial x}\right)_{i-\frac{1}{2},j} = \frac{(ZDT)_{i,j} - (ZDT)_{i-1,j}}{\Delta x} \quad (5.36b)$$

Substitution of Equation 5.36 into 5.35 and rearrangement of the terms yields

$$\left[\frac{\partial}{\partial x}D_{xx}\frac{\partial(ZDT)}{\partial x}\right]_{i,j} = \frac{1}{\Delta x^2}\left\{D_{xx_{i-\frac{1}{2},j}}(ZDT)_{i-1,j} - \left[D_{xx_{i-\frac{1}{2},j}} + D_{xx_{i+\frac{1}{2},j}}\right](ZDT)_{i,j} + D_{xx_{i+\frac{1}{2},j}}(ZDT)_{i+1,j}\right\} \quad (5.37)$$

Similarly,

$$\left[\frac{\partial}{\partial x} D_{xy} \frac{\partial(ZDT)}{\partial y}\right]_{i,j} = \frac{1}{\Delta x}\left\{D_{xy_{i+\frac{1}{2},j}}\left[\frac{\partial(ZDT)}{\partial y}\right]_{i+\frac{1}{2},j}\right.$$

$$\left. - D_{xy_{i-\frac{1}{2},j}}\left[\frac{\partial(ZDT)}{\partial y}\right]_{i-\frac{1}{2},j}\right\} \qquad (5.38)$$

where, by analogy to Equations 5.9 and 5.10,

$$\left[\frac{\partial(ZDT)}{\partial y}\right]_{i+\frac{1}{2},j} = \frac{1}{2}\left\{\left[\frac{\partial(ZDT)}{\partial y}\right]_{i+1,j} + \left[\frac{\partial(ZDT)}{\partial y}\right]_{i,j}\right\} \qquad (5.39a)$$

and

$$\left[\frac{\partial(ZDT)}{\partial y}\right]_{i-\frac{1}{2},j} = \frac{1}{2}\left\{\left[\frac{\partial(ZDT)}{\partial y}\right]_{i,j} + \left[\frac{\partial(ZDT)}{\partial y}\right]_{i-1,j}\right\} \qquad (5.39b)$$

The difference between Equations 5.36 and 5.39 is that the derivative in the first one is with respect to x while the derivative in the second one is with respect to y; therefore, the approximation of each of them takes a different form.

Now, by analogy to Equation 5.8,

$$\left[\frac{\partial(ZDT)}{\partial y}\right]_{i+1,j} = \frac{1}{\Delta y}\left[(ZDT)_{i+1,j+\frac{1}{2}} - (ZDT)_{i+1,j-\frac{1}{2}}\right]$$

$$= \frac{1}{\Delta y}\left\{.5\left[(ZDT)_{i+1,j+1} + (ZDT)_{i+1,j}\right] - .5\left[(ZDT)_{i+1,j} + (ZDT)_{i+1,j-1}\right]\right\}$$

Hence,

$$\left[\frac{\partial(ZDT)}{\partial y}\right]_{i+1,j} = \frac{1}{2\Delta y}\left[(ZDT)_{i+1,j+1} - (ZDT)_{i+1,j-1}\right] \qquad (5.40a)$$

This approximation could also be obtained directly by applying Equation 5.7.

The approximation of the remaining terms of Equation 5.39 is obtained in a similar way as

$$\left[\frac{\partial(ZDT)}{\partial y}\right]_{i,j} = \frac{1}{2\Delta y}\left[(ZDT)_{i,j+1} - (ZDT)_{i,j-1}\right] \tag{5.40b}$$

$$\left[\frac{\partial(ZDT)}{\partial y}\right]_{i-1,j} = \frac{1}{2\Delta y}\left[(ZDT)_{i-1,j+1} - (ZDT)_{i-1,j-1}\right] \tag{5.40c}$$

Equation 5.38 finally takes the form,

$$\left[\frac{\partial}{\partial x} D_{xy} \frac{\partial(ZDT)}{\partial y}\right]_{i,j} = \frac{1}{4\,\Delta x\,\Delta y}\left\{D_{xy_{i+1/2,j}}\left[(ZDT)_{i+1,j+1} - (ZDT)_{i+1,j-1}\right.\right.$$

$$\left. + (ZDT)_{i,j+1} - (ZDT)_{i,j-1}\right] - D_{xy_{i-1/2,j}}\left[(ZDT)_{i,j+1} - (ZDT)_{i,j-1}\right.$$

$$\left.\left. + (ZDT)_{i-1,j+1} - (ZDT)_{i-1,j-1}\right]\right\} \tag{5.41}$$

The introduction of 4.58 into 5.8 leads to

$$\frac{\partial}{\partial x} q_x = \frac{1}{\Delta x}\left[(K_x \frac{\partial \Delta}{\partial x})_{i+1/2,j,k}\right] \tag{5.42}$$

where, by analogy to Equation 5.8,

$$(K_x \frac{\partial s}{\partial x})_{i+1/2,j,k} = K_{x_{i+1/2,j,k}} \frac{s_{i+1,j,k} - s_{i,j,k}}{\Delta x} \tag{5.43a}$$

and

$$(K_x \frac{\partial s}{\partial x})_{i-1/2,j,k} = K_{x_{i-1/2,j,k}} \frac{s_{i,j,k} - s_{i-1,j,k}}{\Delta x} \tag{5.43b}$$

Introduction of Equation 5.43 into 5.42 and rearrangement of terms leads to

$$\frac{\partial}{\partial x}(q_x)_{i,j,k} = \frac{1}{\Delta x^2}\{[K_{x_{i-1/2,j,k}}]\, s_{i-1,j,k} - ([K_{i-1/2,j,k}] + [K_{i+1/2,j,k}])\, s_{i,j,k} + [K_{i+1/2,j,k}]\, s_{i+1,j,k}\} \tag{5.44}$$

The approximation of $\frac{\partial}{\partial z}(q_z)$ is, however, different in form from Equation 5.44 because of the vertical grid size Δz (the thickness of the layers) which is variable. By analogy to Equation 5.42

$$\frac{\partial}{\partial z}(q_z)_{i,j,k} = \frac{1}{\Delta z_{i,j,k}}\{(K_z \frac{\partial s}{\partial x})_{i,j,k+1/2} - (K_z \frac{\partial s}{\partial z})_{i,j,k-1/2}\} \tag{5.45}$$

where

$$(K_z \frac{\partial s}{\partial z})_{i,j,k+1/2} = K_{z_{i,j,k+1/2}} \frac{s_{i,j,k+1} - s_{i,j,k}}{\Delta z_{i,j,k+1/2}} \tag{5.46a}$$

$$(K_z \frac{\partial s}{\partial z})_{i,j,k-1/2} = K_{z_{i,j,k-1/2}} \frac{s_{i,j,k} - s_{i,j,k-1}}{\Delta z_{i,j,k-1/2}} \tag{5.46b}$$

$\Delta z_{i,j,k} = B_{i,j,k}$ = thickness of layer k at $P_{i,j,k}$

$$\Delta z_{i,j,k+1/2} = \frac{1}{2}(B_{i,j,k+1} + B_{i,j,k}) \tag{5.47a}$$

$$\Delta z_{i,j,k-1/2} = \frac{1}{2}(B_{i,j,k} + B_{i,j,k-1}) \tag{5.47b}$$

Equation 5.45 finally takes the form

$$\frac{\partial}{\partial z}(q_z)_{i,j,k} = \frac{1}{B_{i,j,k}}\{[K_z]_{i,j,k+\frac{1}{2}} \frac{(s_{i,j,k+1} - s_{i,j,k})}{.5(B_{i,j,k+1} + B_{i,j,k})} - [K_z]_{i,j,k-\frac{1}{2}} \frac{(s_{i,j,k} - s_{i,j,k-1})}{.5(B_{i,j,k} - B_{i,j,k-1})}\} \quad (5.48)$$

Replacement of the derivatives in the flow and the transport equations by their appropriate finite-difference analogs will provide the numerical model of the upcoming problem.

5.4 The Numerical Analog of the Flow Model

The mathematical model of the flow in the aquifer system is represented by Equation 4.92:

$$\frac{\partial}{\partial x} q_x + \frac{\partial}{\partial y} q_y + \frac{\partial}{\partial z} q_z + w(x,y,z,t) + \frac{\partial}{\partial x} q_x + \frac{\partial}{\partial y} q_y + \frac{\partial}{\partial z} q_z + w(x,y,z,t) = S_o \frac{\partial \Delta}{\partial t} \quad (5.49)$$

Replacing the derivatives in Equation 5.49 by their appropriate finite-difference analogs, and rearranging terms yields:

$$[\frac{K_{x_{i-\frac{1}{2},j,k}}}{\Delta x^2}]_k s_{i-1,j,k} - ([\frac{K_{x_{i-\frac{1}{2},j,k}}}{\Delta x^2}] + [\frac{K_{x_{i+\frac{1}{2},j,k}}}{\Delta x^2}])s_{i,j,k} + [\frac{K_{x_{i+\frac{1}{2},j,k}}}{\Delta x^2}]s_{i+1,j,k}$$

$$+ [\frac{K_{y_{i,j-\frac{1}{2},k}}}{\Delta y^2}]s_{i,j-1,k} - ([\frac{K_{y_{i,j-\frac{1}{2},k}}}{\Delta y^2}] + [\frac{K_{y_{i+\frac{1}{2},j,k}}}{\Delta y^2}])s_{i,j,k} + [\frac{K_{y_{i,j+\frac{1}{2},k}}}{\Delta y}]s_{i,j+1,k}$$

$$+\frac{1}{B_{i,j,k}}\left\{\left[K_{z_{i,j,k+\frac{1}{2}}}\right]\frac{(s_{i,j,k+1}-s_{i,j,k})}{.5(B_{i,j,k+1}+B_{i,j,k})}\right.$$

$$\left.-\left[K_{z_{i,j,k-\frac{1}{2}}}\right]\frac{(s_{i,j,k}-s_{i,j,k-1})}{.5(B_{i,j,k}+B_{i,j,k-1})}\right\}$$

$$+\frac{Q_{i,j,k}}{\Delta x\cdot\Delta y\cdot B_{i,j,k}}=S_{o_{i,j,k}}\left(\frac{2}{\Delta t}\right)(s^{n+\frac{1}{2}}_{i,j,k}-s^{n}_{i,j,k}) \qquad (5.50)$$

where $Q_{i,j,k}$ is the pumping rate at a producing well located at point $P_{i,j,k}$. Evidently, in zones other than the pumpage zone, $Q_{i,j,k}$ is zero. Assuming that $\Delta x = \Delta y$ and replacing the subscript k by the initial of the concerned layer (e.g., $sL_{i,j}$ for the drawdown in the lower layer at nodal point $P_{i,j}$; $BS_{i,j}$ for the thickness of the saltwater layer at $P_{i,j}$; $KPU_{z_{i,j}}$ for the vertical hydraulic conductivity between the pumpage layer and the upper layer; etc.), the flow equation can be written for each individual layer as follows:

(a) Upper layer

$$\left[\frac{KU_{x_{i-\frac{1}{2},j}}}{\Delta x^2}\right]sU_{i-1,j}-\left(\left[\frac{KU_{x_{i-\frac{1}{2},j}}}{\Delta x^2}\right]+\left[\frac{KU_{x_{i+\frac{1}{2},j}}}{\Delta x^2}\right]\right)sU_{i,j}$$

$$+\left[\frac{KU_{x_{i+\frac{1}{2},j}}}{\Delta x^2}\right]sU_{i+1,j}+\left[\frac{KU_{y_{i,j-\frac{1}{2}}}}{\Delta x^2}\right]sU_{i,j-1}-\left(\left[\frac{KU_{y_{i,j-\frac{1}{2}}}}{\Delta x^2}\right]\right.$$

$$\left.+\left[\frac{KU_{y_{i,j+\frac{1}{2}}}}{\Delta x^2}\right]\right)sU_{i,j}+\left[\frac{KU_{y_{i,j+\frac{1}{2}}}}{\Delta x^2}\right]sU_{i,j+1}$$

$$+\left[\frac{K'_{z_{i,j}}}{BU_{i,j}}\right]\frac{(sH_{i,j}-sU_{i,j})}{B'_{i,j}}-\left[\frac{KPU_{z_{i,j}}}{BU_{i,j}}\right]\frac{(sU_{i,j}-sP_{i,j})}{.5(BU_{i,j}+BP_{i,j})}$$

$$=\frac{2S_{oU_{i,j}}}{\Delta t}(sU^{n+\frac{1}{2}}_{i,j}-sU^{n}_{i,j}) \qquad (5.51)$$

where

KU_x = the upper layer hydraulic conductivity in the x direction

KU_y = the upper layer hydraulic conductivity in the y direction

sU = the drawdown in the upper layer

K'_z = vertical hydraulic conductivity in the semi-confining layer on the top of the upper layer

B' = thickness of the semi-confining layer (L)

sH = drawdown in the water table

KPU_z = vertical hydraulic conductivity between the pumpage and the upper layers

sP = drawdown in the pumpage layer

S_{oU} = specific storage coefficient in the upper layer

BU = thickness of the upper zone

BP = thickness of the pumpage zone

(b) Pumpage layer

$$\left[\frac{KPx_{i-\frac{1}{2},j}}{\Delta x^2}\right] sP_{i-1,j} - \left(\left[\frac{KPx_{i-\frac{1}{2},j}}{\Delta x^2}\right] + \left[\frac{KPx_{i+\frac{1}{2},j}}{\Delta x^2}\right]\right) sP_{i,j} + \left[\frac{KPx_{i+\frac{1}{2},j}}{\Delta x^2}\right] sP_{i+1,j}$$

$$+ \left[\frac{KPy_{i,j-\frac{1}{2}}}{\Delta x^2}\right] sP_{i,j-1} - \left(\left[\frac{KPy_{i,j-\frac{1}{2}}}{\Delta x^2}\right] + \left[\frac{KPy_{i,j+\frac{1}{2}}}{\Delta x^2}\right]\right) sP_{i,j} + \left[\frac{KPy_{i,j+\frac{1}{2}}}{\Delta x^2}\right] sP_{i,j+1}$$

$$+ \frac{1}{BP_{i,j}}\left\{KPU_{z_{i,j}} \frac{(sU_{i,j} - sP_{i,j})}{.5(BU_{i,j} + BP_{i,j})} - KLP_{z_{i,j}} \frac{(sP_{i,j} + sL_{i,j})}{.5(BP_{i,j} + BL_{i,j})}\right\}$$

$$+ \frac{Q_{i,j}}{\Delta x^2 \; BP_{i,j}} = \frac{2S_{op_{i,j}}}{\Delta t}\left(sP_{i,j}^{n+\frac{1}{2}} - sP_{i,j}^{n}\right) \qquad (5.52)$$

where

KP_x = the pumpage layer hydraulic conductivity in x direction

KP_y = the pumpage layer hydraulic conductivity in y direction

KPU_z = vertical hydraulic conductivity between the pumpage zone and the upper zone

KLP_z = vertical hydraulic conductivity between the lower zone and the pumpage zone

sL = drawdown in the lower zone

BL = thickness of the lower zone (which in fact is equal to the elevation Z_L)

S_{op} = specific storage coefficient in the pumpage zone

(c) Lower layer

$$\left[\frac{KL_{x_{i-1/2,j}}}{\Delta x^2}\right] sL_{i-1,j} - \left(\left[\frac{KL_{x_{i-1/2,j}}}{\Delta x^2}\right] + \left[\frac{KL_{x_{i+1/2,j}}}{\Delta x^2}\right]\right) sL_{i,j}$$

$$+ \left[\frac{KL_{x_{i+1/2,j}}}{\Delta x^2}\right] sL_{i+1,j} + \left[\frac{KL_{y_{i,j-1/2}}}{\Delta x^2}\right] sL_{i,j-1} - \left(\left[\frac{KL_{y_{i,j-1/2}}}{\Delta x^2}\right]\right.$$

$$\left. + \left[\frac{KL_{y_{i,j+1/2}}}{\Delta x^2}\right]\right) sL_{i,j} + \left[\frac{KL_{y_{i,j+1/2}}}{\Delta x^2}\right] sL_{i,j+1}$$

$$+ \left[\frac{KLP_{z_{i,j}}}{BL_{i,j}}\right] \frac{sP_{i,j} - sL_{i,j}}{.5(BP_{i,j} + BL_{i,j})} - \left[\frac{KLS_{z_{i,j}}}{BL_{i,j}}\right] \frac{(sL_{i,j} - sS_{i,h})}{.5(BL_{i,j} + BS_{i,j})}$$

$$= \frac{2S_{0L_{i,j}}}{\Delta t} (sL^{n+1/2}_{i,j} - sL^{n}_{i,j}) \qquad (5.53)$$

where

KL_x = lower zone hydraulic conductivity in x direction

KL_y = lower zone hydraulic conductivity in y direction

KLS_z = vertical hydraulic conductivity between the saltwater zone and the lower zone

sS = drawdown in the saltwater zone in terms of freshwater as fluid of reference (i.e., drawdown obtained if the saltwater was replaced by freshwater).

BS = thickness of the saltwater zone

S_{oL} = specific storage coefficient in the lower zone

(d) Saltwater layer

$$\left[\frac{KS_{x_{i-1/2,j}}}{\Delta x^2}\right] sS_{i-1,j} - \left(\left[\frac{KS_{x_{i-1/2,j}}}{\Delta x^2}\right] + \left[\frac{KS_{i+1/2,j}}{\Delta x^2}\right]\right) sS_{i,j}$$

$$+ \left[\frac{KS_{x_{i+1/2,j}}}{\Delta x^2}\right] sS_{i+1,j} + \left[\frac{KS_{y_{i,j-1/2}}}{\Delta x^2}\right] sS_{i,j-1} - \left(\left[\frac{KS_{y_{i,j-1/2}}}{\Delta x^2}\right]\right.$$

$$\left. + \left[\frac{KS_{y_{i,j+1/2}}}{\Delta x^2}\right]\right) sS_{i,j} + \left[\frac{KS_{y_{i,j+1/2}}}{\Delta x^2}\right] sS_{i,j+1}$$

$$+ \left[\frac{KSL_{z_{i,j}}}{BS_{i,j}}\right] \frac{(sS_{i,j} - sL_{i,j})}{.5(BU_{i,j} + BS_{i,j})} = \frac{2S_{oS_{i,j}}}{\Delta t} (sS^{n+1/2}_{i,j} - sS^{n}_{i,j}) \qquad (5.54)$$

where

KS_x = saltwater hydraulic conductivity in x direction

KS_y = saltwater hydraulic conductivity in y direction

S_{oS} = specific storage coefficient in the saltwater zone

In the derivation of Equations 5.51, 5.53, and 5.54, the sink term vanishes because there is no pumping in layers other than the pumpage zone.

5.5 The Numerical Analog of the Transport Model

The mathematical model of the transport process in the aquifer system is represented by the following equations (Equations 4.69, 4.84 and 4.99)

$$\frac{\partial}{\partial x}\left(q_x \frac{c}{c_s}\right) + \frac{\partial}{\partial y}\left(q_y \frac{c}{c_s}\right) + \frac{\partial}{\partial z}\left(q_z \frac{c}{c_s}\right) + \left(\frac{c}{c_s}\right)w + n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) = \left(\frac{c}{c_s}\right) S_o \frac{\partial s}{\partial t} \qquad (5.55)$$

where $(\frac{c}{c_s})w$ is a sink term representing the amount of salty water leaving the pumpage zone (from the well).

$$n\frac{\partial Z_b}{\partial t} + Z_b(S_o\frac{\partial s}{\partial t}) = -\frac{\partial}{\partial x}(q_x Z_b) - \frac{\partial}{\partial y}(q_y Z_b) + q_{z_o} - \frac{L'(0)}{\delta}\left[D_{xz}\frac{\partial Z_b}{\partial x} + D_{yz}\frac{\partial Z_b}{\partial y} - D_{zz}\right] \tag{5.56}$$

and

$$n\frac{\partial}{\partial t}(ZDT) - ZDT(S_o\frac{\partial s}{\partial t}) = \frac{\partial}{\partial x}D_{xx}\frac{\partial}{\partial x}(ZDT) + \frac{\partial}{\partial x}D_{xy}\frac{\partial}{\partial y}(ZDT) - \frac{\partial}{\partial x}D_{xz} + \frac{\partial}{\partial y}D_{yx}\frac{\partial}{\partial x}(ZDT) + \frac{\partial}{\partial y}D_{yy}\frac{\partial}{\partial y}(ZDT) - \frac{\partial}{\partial y}D_{yz} - \frac{\partial}{\partial x}[q_x(ZDT)] - \frac{\partial}{\partial y}[q_y(ZDT)] + q_{z_o} \tag{5.57}$$

Introducing 4.95 into 5.55 and replacing the derivatives by their appropriate finite-difference analogs leads to

$$\frac{1}{\Delta x}\left[q_{x_{i+\frac{1}{2},j}}\begin{bmatrix}(+)(\frac{c}{c_s})_{i,j}\\(-)(\frac{c}{c_s})_{i+1,j}\end{bmatrix} - q_{x_{i-\frac{1}{2},j}}\begin{bmatrix}(+)(\frac{c}{c_s})_{i-1,j}\\(-)(\frac{c}{c_s})_{i,j}\end{bmatrix}\right.$$

$$+\frac{1}{\Delta y}\left[q_{y_{i,j+\frac{1}{2}}}\begin{bmatrix}(+)(\frac{c}{c_s})_{i,j}\\(-)(\frac{c}{c_s})_{i,j+1}\end{bmatrix} - q_{y_{i,j+\frac{1}{2}}}\begin{bmatrix}(+)(\frac{c}{c_s})_{i,j-1}\\(-)(\frac{c}{c_s})_{i,j}\end{bmatrix}\right.$$

$$+\frac{1}{BP_{i,j}}\left[\int_{z_L}^{z_t}n\frac{\partial}{\partial t}(\frac{c}{c_s})dz\right]_{i,j} - \frac{Q_{p_{i,j}}}{BP\cdot\Delta x\cdot\Delta y}(\frac{c}{c_s})_{i,j} + \frac{2n}{\Delta t}\left[(\frac{c}{c_s})^{n+\frac{1}{2}}_{i,j} - (\frac{c}{c_s})^{n}_{i,j}\right]$$

$$= \left[\frac{2S_o}{\Delta t}(sp^{n+\frac{1}{2}}_{i,j} - sp^{n})\right](\frac{c}{c_s})_{i,j} \tag{5.58}$$

Defining

$$ZDP = \int_{z_L}^{z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dZ \tag{5.59}$$

which is evaluated using Equations 4.86 through 4.88, assuming that $\Delta x = \Delta y$, multiplying both sides of 5.58 by Δx and rearranging the terms yields

$$\frac{2n\Delta x}{\Delta t}\left[\left(\frac{c}{c_s}\right)_{i,j}^{n+\frac{1}{2}} - \left(\frac{c}{c_s}\right)_{i,j}^{n}\right] = q^p_{x_{i-\frac{1}{2},j}}\left[\frac{(+)\left(\frac{c}{c_s}\right)_{i-1,j}}{(-)\left(\frac{c}{c_s}\right)_{i,j}}\right] - q^p_{x_{i+\frac{1}{2}}}\left[\frac{(+)\left(\frac{c}{c_s}\right)_{i,j}}{(-)\left(\frac{c}{c_s}\right)_{i+1,j}}\right]$$

$$+ q^p_{y_{i,j-\frac{1}{2}}}\left[\frac{(+)\left(\frac{c}{c_s}\right)_{i,j-1}}{(-)\left(\frac{c}{c_s}\right)_{i,j}}\right] - q^p_{y_{i,j+\frac{1}{2}}}\left[\frac{(+)\left(\frac{c}{c_x}\right)_{i,j}}{(-)\left(\frac{c}{c_s}\right)_{i,j+1}}\right] + \left(\frac{ZDP}{\delta P}\right)_{i,j}$$

$$- \frac{Q_{p_{i,j}}}{BP\cdot\Delta x}\left(\frac{c}{c_s}\right)_{i,j} + \frac{2S_0}{\Delta t}\left(sP^{n+\frac{1}{2}}_{i,j} - sP^{n}_{i,j}\right)\left(\frac{c}{c_s}\right)_{i,j} \tag{5.60}$$

which is the numerical model of the chloride concentration in the pumpage zone.

Replacing the derivatives in Equation 5.56 by their appropriate finite-difference analogs leads to:

$$\frac{2}{\Delta t}\left[n\left(Z^{n+\frac{1}{2}}_{b_{i,j}} - Z^{n}_{b_{i,j}}\right) - S_{oL_{i,j}}\left(sL^{n+\frac{1}{2}}_{i,j} - sL^{n}_{i,j}\right) Z_{b_{i,j}}\right] = q_{z_{o_{i,j}}}$$

$$+ \frac{1}{\Delta x}\left\{q^L_{x_{i-\frac{1}{2},j}}\left[\frac{(+)\left(Z_{b_{i-1,j}}\right)}{(-)\left(Z_{b_{i,j}}\right)}\right] - q^L_{x_{i+\frac{1}{2},j}}\left[\frac{(+)\left(Z_{b_{i,j}}\right)}{(-)\left(Z_{b_{i+1,j}}\right)}\right]\right\} + \frac{1}{\Delta y}\left\{q^L_{y_{i,j-\frac{1}{2}}}\right.$$

$$\left.\left[\frac{(+)\left(Z_{b_{i,j-1}}\right)}{(-)\left(Z_{b_{i,j}}\right)}\right] - q^L_{y_{i,j+\frac{1}{2}}}\left[\frac{(+)\left(Z_{b_{i,j}}\right)}{(-)\left(Z_{b_{i,j+1}}\right)}\right] - \frac{.5\ L'(0)}{\delta_{i,j}}\right\}\left\{\frac{1}{\Delta x}\left[D_{xz_{i+\frac{1}{2},j}}\right.\right.$$

$$(Z_{b_{i+1,j}} - Z_{b_{i,j}}) + D_{xz_{i-\frac{1}{2},j}}(Z_{b_{i,j}} - Z_{b_{i-1,j}})] + \frac{1}{\Delta y}[D_{yz_{i,j+\frac{1}{2}}}$$

$$(Z_{b_{i,j+1}} - Z_{b_{i,j}}) + D_{yz_{i,j-\frac{1}{2}}}(Z_{b_{i,j}} - Z_{b_{i,j-1}})] - 2\,D_{zz_{i,j}}\} \qquad (5.61)$$

Assuming that $\Delta x = \Delta y$, multiplying both sides of 5.61 by Δx and rearranging the terms leads to

$$\frac{2\Delta x}{\Delta t}[n(Z^{n+\frac{1}{2}}_{b_{i,j}} - Z^{n}_{b_{i,j}}) - S_{oL_{i,j}}(sL^{n+\frac{1}{2}}_{i,j} - sL^{n}_{i,j})\,Z_{b_{i,j}}] = \Delta x\, q_{z_{o_{i,j}}}$$

$$+ q^{L}_{x_{i-\frac{1}{2},j}}[{}^{(+)(Z_{b_{i-1,j}})}_{(-)(Z_{b_{i,j}})}] - q^{L}_{x_{i+\frac{1}{2},j}}[{}^{(+)(Z_{b_{i,j}})}_{(-)(Z_{b_{i+1,j}})}]$$

$$+ q^{L}_{y_{i,j-\frac{1}{2}}}[{}^{(+)(Z_{b_{i,j-1}})}_{(-)(Z_{b_{i,j}})}] - q^{L}_{y_{i,j+\frac{1}{2}}}[{}^{(+)(Z_{b_{i,j}})}_{(-)(Z_{b_{i,j+1}})}] - \frac{.5\,L'(0)}{\delta_{i,j}}$$

$$\{D_{xz_{i+\frac{1}{2},j}}(Z_{b_{i+1,j}} - Z_{b_{i,j}}) + D_{xz_{i-\frac{1}{2},j}}(Z_{b_{i,j}} - Z_{b_{i-1,j}}) + D_{yz_{i,j+\frac{1}{2}}}$$

$$(Z_{b_{i,j+1}} - Z_{b_{i,j}}) + D_{yz_{i,j-\frac{1}{2}}}(Z_{b_{i,j}} - Z_{b_{i,j-1}}) - 2\Delta x\, D_{zz_{i,j}}\} \qquad (5.62)$$

which is the numerical model for the growth of the saltwater mound.

Replacing the derivatives in Equation 5.57 by their appropriate finite-difference analogs leads to

$$\frac{2n}{\Delta t^{L}}[(ZDT)^{n+\frac{1}{2}}_{i,j} - (ZDT)^{n}_{i,j}] - [\frac{2}{\Delta t}S_{OL_{i,j}}(sL^{n+\frac{1}{2}}_{i,j} - sL^{n}_{i,j})](ZDT)_{i,j}$$

$$= \frac{1}{\Delta x^{2}}\{D_{xx_{i-\frac{1}{2},j}}(ZDT)_{i-1,j} - [D_{xx_{i-\frac{1}{2},j}} + D_{xx_{i+\frac{1}{2},j}}](ZDT)_{i,j}$$

$$+ D_{xx_{i+\frac{1}{2},j}}(ZDT)_{i+1,j}\} + \frac{.25}{\Delta x\,\Delta y}[D_{xy_{i+\frac{1}{2},j}}[(ZDT)_{i+1,j+1} - (ZDT)_{i+1,j+1}$$

$$+ (ZDT)_{i,j+1} - (ZDT)_{i,j-1}] - D_{xy_{i-\frac{1}{2},j}}[ZDT_{i,j+1} - (ZDT)_{i,j-1}$$

$$+ (ZDT)_{i-1,j+1} - (ZDT)_{i-1,j-1}] + D_{yx_{i,j+\frac{1}{2}}}[(ZDT)_{i+1,j+1} - (ZDT)_{i-1,j+1}$$

$$+ (ZDT)_{i+1,j} - (ZDT)_{i-1,j}] - D_{yx_{i,j-\frac{1}{2}}}[(ZDT)_{i+1,j} - (ZDT)_{i-1,j}$$

$$+ (ZDT)_{i+1,j-1} - (ZDT)_{i-1,j-1}]\} - \frac{1}{\Delta x}(D_{xz_{i+\frac{1}{2},j}} - D_{xz_{i-\frac{1}{2},j}}$$

$$- \frac{1}{\Delta y}(D_{yz_{i,j+\frac{1}{2}}} - D_{yz_{i,j-\frac{1}{2}}}) + \frac{1}{\Delta y^2}[D_{yy_{i,j-\frac{1}{2}}}(ZDT)_{i,j-1}$$

$$- [D_{yy_{i,j-\frac{1}{2}}} + D_{xy_{i,j+\frac{1}{2}}}](ZDT)_{i,j} + D_{yy_{i,j+\frac{1}{2}}}(ZDT)_{i,j+1}\}$$

$$+ \frac{1}{\Delta x}[q^L_{x_{i-\frac{1}{2},j}}[\begin{matrix}(+)(ZDT)_{i-1,j}\\(-)(ZDT)_{i,j}\end{matrix}] - q^L_{x_{i+\frac{1}{2},j}}[\begin{matrix}(+)(ZDT)_{i,j}\\(-)(ZDT)_{i+1,j}\end{matrix}]\}$$

$$+ \frac{1}{\Delta y}[q^L_{y_{i,j-\frac{1}{2}}}[\begin{matrix}(+)(ZDT)_{i,j-1}\\(-)(ZDT)_{i,j}\end{matrix}] - q^L_{y_{i,j+1}}[\begin{matrix}(+)(ZDT)_{i,j}\\(-)(ZDT)_{i,j}\end{matrix}]\} + q_{ZO_{i,j}} \qquad (5.63)$$

Again, assuming that $\Delta x = \Delta y$, multiplying by Δx^2, and rearranging the terms leads to

$$\frac{2n\Delta x^2}{\Delta t}[(ZDT)^{n+\frac{1}{2}}_{i,j} - (ZDT)^n_{i,j}] - [\frac{2\Delta x^2}{\Delta t}S_{OL_{i,j}}(sL^{n+\frac{1}{2}}_{i,j} - sL^n_{i,j})](ZDT)_{i,j}$$

$$= [D_{xx_{i-\frac{1}{2},j}} - .25(D_{yx_{i,j+\frac{1}{2}}} - D_{yx_{i,j-\frac{1}{2}}})](ZDT)_{i-1,j} - [D_{xx_{i-\frac{1}{2},j}}$$

$$+ D_{xx_{i+\frac{1}{2},j}}](ZDT)_{i,j} + [D_{xx_{i+\frac{1}{2},j}} + .25(D_{yx_{i,j+\frac{1}{2}}} - D_{yx_{i,j-\frac{1}{2}}})](ZDT)_{i+1,j}$$

$$+ \Delta x\{q^L_{x_{i-\frac{1}{2},j}}[\begin{matrix}(+)(ZDT)_{i-1,j}\\(-)(ZDT)_{i,j}\end{matrix}] - q^L_{x_{i+\frac{1}{2},j}}[\begin{matrix}(+)(ZDT)_{i,j}\\(-)(ZDT)_{i+1,j}\end{matrix}]\} + [D_{yy_{i,j-\frac{1}{2}}}$$

$$- .25(D_{xy_{i+\frac{1}{2},j}} - D_{xy_{i-\frac{1}{2},j}})](ZDT)_{i,j-1} - [D_{yy_{i,j-\frac{1}{2}}} + D_{yy_{i,j+\frac{1}{2}}}](ZDT)_{i,j}$$

$$+ [D_{yy_{i,j+\frac{1}{2}}} + .25(D_{xy_{i+\frac{1}{2},j}} - D_{xy_{i-\frac{1}{2},j}})](ZDT)_{i,j+1}$$

$$+ \Delta x\{q^{L}_{y_{i,j-\frac{1}{2}}}[(+)(ZDT)_{i,j-1} - (-)(ZDT)_{i,j}] - q^{L}_{y_{i,j+\frac{1}{2}}}[(+)(ZDT)_{i,j} - (-)(ZDT)_{i,j+1}]\}$$

$$+ .25\{D_{xy_{i+\frac{1}{2},j}}[(ZDT)_{i+1,j+1} - (ZDT)_{i+1,j-1}]$$

$$- D_{xy_{i-\frac{1}{2}}}[(ZDT)_{i-1,j+1} - (ZDT)_{i-1,j-1}] + D_{yx_{i,j+\frac{1}{2}}}[(ZDT)_{i+1,j+1}$$

$$- (ZDT)_{i-1,j+1}] - D_{yx_{i,j-\frac{1}{2}}}[(ZDT)_{i+1,j-1} - (ZDT)_{i-1,j-1}]\}$$

$$- \Delta x(D_{xz_{i+\frac{1}{2},j}} - D_{xz_{i-0},j} + D_{yz_{i,j+\frac{1}{2}}} - D_{yz_{i,j-\frac{1}{2}}}) + \Delta x^2 q_{Z_0} \qquad (5.64)$$

and from 4.83,

$$\delta_{i,j} = [(ZDT)_{i,j} - Z_{b_{i,j}}]/(\int_0^j m(n)dn)$$

Equations 5.64 and 5.65 are the numerical model for the development of the transition zone. Equation 5.65 together with 5.61 and 5.64 represent the transport model in the lower zone.

5.6 Method of Solving the Finite-Difference Equations of the Upconing Problem

Several methods can be used to solve the three-dimensional finite-difference equations representing the numerical model of the upconing problem (Equations 5.51 through 5.54, 5.61, 5.64, and 5.65). However, due to the complexity of the problem and the flexibility of the ADI methods, the latter seems to be the more appropriate method to be used

for the solution of the equations developed in the previous paragraphs.

The two-step algorithm proposed by Peaceman and Rachford (1955) for the solution of two space-variables problem is as follows:

$$\Delta_x^2 U_{i,j}^{n+\frac{1}{2}} + \Delta_y^2 U_{i,j}^{n} = \frac{U_{i,j}^{n+\frac{1}{2}} - U_{i,j}^{n}}{\frac{\Delta t}{2}} \tag{5.66a}$$

$$\Delta_x^2 U_{i,j}^{n+\frac{1}{2}} + \Delta_y^2 U_{i,j}^{n+1} = \frac{U_{i,j}^{n+1} - U_{i,j}^{n+\frac{1}{2}}}{\frac{\Delta t}{2}} \tag{5.66b}$$

where

$$\Delta_x^2 U_{i,j} = \left(\frac{\partial^2 U}{\partial x^2}\right)_{i,j} \tag{5.67a}$$

$$\Delta_y^2 U_{i,j} = \left(\frac{\partial^2 U}{\partial y^2}\right)_{i,j} \tag{5.67b}$$

The method has been applied to two-dimensional transient groundwater flow where equation 5.67 takes the form

$$\Delta_x^2 U_{i,j} = \left(\frac{\partial}{\partial x} T_x \frac{\partial \phi}{\partial x}\right)_{i,j} \tag{5.68a}$$

$$\Delta_y^2 U_{i,j} = \left(\frac{\partial}{\partial y} T_y \frac{\partial \phi}{\partial y}\right)_{i,j} \tag{5.68b}$$

While this method is unconditionally stable for two-dimensional problems, there is a restriction on its stability when applied to problems with three space variables. Peaceman (1977) shows that the condition of stability is

$$\frac{\Delta t'}{(\Delta x')^2} < \frac{3}{2} \tag{5.69}$$

where

$\Delta t'$ = dimensionless time interval

$\Delta x'$ = dimensionless space interval.

Douglas and Rachford (1956) developed the following three-dimensional, unconditionally stable ADI algorithm

$$\delta_x^2 U^{n+1/3} + \delta_y^2 U^n + \delta_y^2 U^n = \frac{U^{n+1/3} - U^n}{\Delta t} \tag{5.70a}$$

$$\delta_x^2 U^{n+1/3} + \delta_y^2 U^{n+2/3} + \delta_z^2 U^n = \frac{U^{n+2/3} - U^n}{\Delta t} \tag{5.70b}$$

$$\delta_x^2 U^{n+1/3} + \delta_y^2 U^{n+2/3} + \delta_z^2 U^{n+1} = \frac{U^{n+1} - U^n}{\Delta t} \tag{5.70c}$$

where

$U = u_{i,j,k}$; the subscripts i, j, and k are dropped just for the simplicity of the presentation.

Equation 5.70 is a three-step algorithm and can be transformed into

$$\delta_x^2 U^{n+1/3} + \delta_y^2 U^n + \delta_z^2 U^n = \frac{U^{n+1/3} - U^n}{\Delta t} \tag{5.71a}$$

$$\delta_y^2 U^{n+1} = \delta_z^2 U^n + \frac{U^{n+1} - U^{n+2/3}}{\Delta t} \tag{5.71b}$$

$$\delta_z^2 U^{n+1} = \delta_z^2 U^n + \frac{U^{n+1} - U^{n+2/3}}{\Delta t} \tag{5.71c}$$

Peaceman (1977), in an analogy to methods using "predictions" and "corrections," suggested that the second and third (5.71b and 5.71c) might be considered as "corrections" to the first (5.71a).

Brian (1961) suggested the following four-step calculation algorithm:

$$\delta_x^2 U^{n+1/6} + \delta_y^2 U^n + \delta_z U^n = \frac{U^{n+1/6} - U^n}{\frac{\Delta t}{2}} \tag{5.72a}$$

$$\Delta_y^2 U^{n+2/6} = \Delta_y^2 U^n + \frac{U^{n+2/6} - U^{n+1/6}}{\frac{\Delta t}{2}} \tag{5.72b}$$

$$\Delta_z U^{n+1/2} = \Delta_z^2 U^n + \frac{U^{n+1} - U^{n+2/6}}{\frac{\Delta t}{2}} \tag{5.72c}$$

$$U^{n+1} = 2U^{n+1/2} - U^n \tag{5.72d}$$

Douglas (1962) proposed another three step algorithm which in its final form can be related to the well known Crank-Nicolson implicit method:

$$\frac{1}{2}\Delta_x^2(U^{n+1/3} + U^n) + \frac{1}{2}\Delta_y^2(U^{n+2/3} + U^n) + \frac{1}{2}(U^{n+1} + U^n) = \frac{U^{n+1} - U^n}{\Delta t} \tag{5.73}$$

where $U^{n+1/3}$ and $U^{n+2/3}$ are actually the first and second estimates of U^{n+1}. The algorithm can be written as:

$$\frac{1}{2}\Delta_x^2(U^{n+1/3} + U^n) + \Delta_y^2 U^n + \Delta_z^2 U^n = \frac{U^{n+1/3} - U^n}{\Delta t} \tag{5.74a}$$

$$\frac{1}{2}\Delta_x^2 U^{n+2/3} = \frac{1}{2}\Delta_y^2 U^n + \frac{U^{n+1/3} - U^{n+1/3}}{\Delta t} \tag{5.74b}$$

$$\frac{1}{2}\Delta_z^2 U^{n+1} = \frac{1}{2}\Delta_z^2 U^n + \frac{U^{n+1} - U^{n+2/3}}{\Delta t} \tag{5.74c}$$

The intermediate time level in Equations 5.71, 5.72, and 5.74 are misleading. The three algorithms can be considered an iterative method with a fixed number of iterations (Brian 1961). In that sense, $U^{n+1/3}$ and $U^{n+2/3}$ in Equations 5.71 and 5.74 are the first and second estimates of U^{n+1}; $U^{n+1/6}$ and $U^{n+2/6}$ in 5.72 are the first and second estimates of $U^{n+1/2}$. Furthermore, assuming that

$$U^{n+1/6} = \frac{1}{2}(U^{n+1/3} + U^{n}) \tag{5.75a}$$

$$U^{n+2/6} = \frac{1}{2}(U^{n+2/3} + U^{n}) \tag{5.75b}$$

$$U^{n+1/2} = \frac{1}{2}(U^{n+1} + U^{n}) \tag{5.75c}$$

It follows that

$$U^{n+1/3} = 2U^{n+1/6} - U^{n} \tag{5.76a}$$

$$U^{n+2/3} = 2U^{n+2/6} - U^{n} \tag{5.76b}$$

$$U^{n+1} = 2U^{n+1/2} - U^{n} \tag{5.76c}$$

The introduction of 5.75 into 5.74 shows that 5.72 and 5.74 are equivalent.

Defining

$$F^{n}_{x_i} = \Delta^2_{x_i} U^{n} \tag{5.77}$$

where

$x_i = (x,y,z)$

and

$$F^{*}_{x} = \Delta^2_{x} U^{*} \tag{5.78a}$$

$$F^{**}_{y} = \Delta^2_{y} U^{**} \tag{5.78b}$$

$$F^{***}_{z} = \Delta^2_{z} U^{***} \tag{5.78c}$$

where U*, U**, and U*** are respectively the first, the second and the third estimates of $U^{n+1/2}$ in 5.72; the general form of the three dimensional ADI algorithm can be written as:

$$F_x^* + F_y^n + F_z^n = \frac{2(U^* - U^n)}{\Delta t} \tag{5.80a}$$

$$F_x^* + F_y^{**} + F_z^n = \frac{2(U^{**} - U^n)}{\Delta t} \tag{5.80b}$$

$$F_x^* + F_y^{**} + F_z^{***} = \frac{2(U^{***} - U^n)}{\Delta t} \tag{5.80c}$$

$$U^{n+1} = 2U^{***} - U^n \tag{5.80d}$$

The important characteristic of Equation 5.78 is that

$$F_x^* = f_x(U^*_{i-1,j,k},\ U^*_{i,j,k},\ U^*_{i+1,j,k}) \tag{5.81a}$$

$$F_y^{**} = f_y(U^{**}_{i,j-1,k},\ U^{**}_{i,j,k},\ U^{**}_{i,j+1,k}) \tag{5.81b}$$

$$F_z^{***} = f_z(U^{***}_{i,j,k-1},\ U^{***}_{i,j,k},\ U^{***}_{i,j,k+1}) \tag{5.81c}$$

so that for each iteration (5.80a, 5.80b, 5.80c), the set of equations has the structure of a tri-diagonal matrix of which the solution algorithm is well known and easy to use. When expression 5.81 takes the form

$$F^*_{x_1} = f_{x_1}(U^*_{i-1,j,k},\ U^*_{i,j,k},\ U^*_{i+1,j,k},\ U^*_{\ell_1,m,n}) \tag{5.82a}$$

$$F^{**}_{y_1} = f_{z_1}(U^{**}_{i,j-1,k},\ U^{**}_{i,j,k},\ U^{**}_{i,j+1,k},\ U^{**}_{\ell,m_1,n}) \tag{5.82b}$$

$$F^{***}_{z_1} = f_{z_1}(U^{***}_{i,j,k-1},\ U^{***}_{i,j,k},\ U^{***}_{i,j,k+1},\ U^{***}_{\ell,m,n_1}) \tag{5.82c}$$

so that

$\ell_1 \neq i-1, i, i+1$

$m_1 \neq j-1, j, j+1$

$n_1 \neq k-1, k, k+1$

like in Equation 5.64 due to terms like $\frac{\partial}{\partial x} D_{xy} \frac{\partial}{\partial y} (ZDT)$, additional iterations would be necessary at each computation step. However Equations 5.82 can be rewritten as

$$F^{*}_{x_1} = F^{*}_{xx} + G^{*}_{x} \tag{5.83a}$$

$$F^{**}_{y_1} = F^{**}_{yy} + G^{**}_{y} \tag{5.83b}$$

$$F^{***}_{z_1} = F^{***}_{zz} + G^{***}_{z} \tag{5.83c}$$

with

$$F^{*}_{xx} = f'_x(U^{*}_{i-1,j,k}, U^{*}_{i,j,k}, U^{*}_{i+1,j,k}) \tag{5.84a}$$

$$G^{*}_{x} = g_x(U^{*}_{\ell_1,m,n}) \tag{5.84b}$$

$$F^{**}_{yy} = f'_y(U^{**}_{i,j-1,k}, U^{**}_{i,j,k}, U^{**}_{i,j+1,k}) \tag{5.84c}$$

$$G^{**}_{y} = g_y(U^{**}_{\ell,m_1 n}) \tag{5.84d}$$

$$F^{***}_{zz} = f'_z(U^{***}_{i,j,k-1}, U^{***}_{i,j,k}, U^{***}_{i,j,k+1}) \tag{5.84e}$$

$$G^{***}_{z} = g_z(U^{***}_{\ell,m,n_1}) \tag{5.84f}$$

and the generalized four-step ADI algorithm (Equation 5.80) becomes the following five-step ADI algorithm

$$F^{*}_{xx} + F^{n}_{yy} + F^{n}_{zz} + G^{n}_{x} + G^{n}_{y} + G^{n}_{z} = \frac{2(U^{*}_{i,j,k} - U^{n}_{i,j,k})}{\Delta t} \tag{5.85a}$$

$$F^{*}_{xx} + F^{**}_{yy} + F^{n}_{zz} + G^{n}_{x} + G^{n}_{y} + G^{n}_{z} = \frac{2(U^{**}_{i,j,k} - U^{n}_{i,j,k})}{\Delta t} \tag{5.85b}$$

$$F^{*}_{xx} + F^{**}_{yy} + F^{***}_{zz} + G^{n}_{x} + G^{n}_{y} + G^{n}_{z} = \frac{2(U^{***}_{i,j,k} - U^{n}_{i,j,k})}{\Delta t} \tag{5.85c}$$

$$F^{*}_{xx} + F^{**}_{yy} + F^{***}_{zz} + G^{*}_{x} + G^{**}_{y} + G^{***}_{z} = \frac{2(U^{n+\frac{1}{2}}_{i,j,k} - U^{n}_{i,j,k})}{\Delta t} \tag{5.85d}$$

which can easily be reduced to

$$F^{*}_{xx} + F^{n}_{yy} + F^{n}_{zz} + G^{n}_{x} + G^{n}_{z} = \frac{2(U^{*}_{i,j,k} - U^{n}_{i,j,k})}{\Delta t} \tag{5.86a}$$

$$F^{**}_{yy} = F^{n}_{yy} + \frac{2(U^{**}_{i,j,k} - U^{*}_{i,j,k})}{\Delta t} \tag{5.86b}$$

$$F^{***}_{zz} = F^{n}_{zz} + \frac{2(U^{***}_{i,j,k} - U^{**}_{i,j,k})}{\Delta t} \tag{5.86c}$$

$$G^{*}_{x} + G^{**}_{y} + G^{***}_{z} = G^{n}_{x} + G^{n}_{y} + G^{n}_{z} + \frac{2(U^{n+\frac{1}{2}}_{i,j,k} - U^{***}_{i,j,k})}{\Delta t} \tag{5.86d}$$

Equations 5.80 and 5.86 are used to solve the numerical model of the upconing problem.

The solution of the drawdown is obtained in the following way:

(1) First iteration: computation in x direction

(a) Upper zone

$$-[\frac{KU_{x_{i-\frac{1}{2},j}}}{\Delta x^2}]sU^{*}_{i-1,j} + [[\frac{KU_{x_{i-\frac{1}{2},j}}}{\Delta x^2}] + [\frac{KU_{x_{i+\frac{1}{2},j}}}{\Delta x^2}]$$

$$+ \frac{2}{\Delta t}S_{oU_{i,j}}\}sU^{*}_{i,j} - [\frac{KU_{x_{i+\frac{1}{2},j}}}{\Delta x^2}]sU^{*}_{i+1,j} = [\frac{KU_{y_{i,j-\frac{1}{2}}}}{\Delta x^2}]sU^{n}_{i,j-1}$$

$$- \{[\frac{KU_{y_{i,j-1/2}}}{\Delta x^2}] + [\frac{KU_{y_{i,j+1/2}}}{\Delta x^2}]\} sU^n_{i,j} + [\frac{KU_{y_{i,j+1/2}}}{\Delta x^2}] sU^n_{i,j+1}$$

$$+ [\frac{K'_{z_{i,j}}}{BU_{i,j}}] \frac{(sH^n_{i,j} - sU^n_{i,j})}{B'_{i,j}} - 2[\frac{KPU_{z_{i,j}}}{BU_{i,j}}] \frac{(sU^n_{i,j} - sP^n_{i,j})}{(BU_{i,j} + BP_{i,j})}$$

$$+ [\frac{2}{\Delta t} S_{OU_{i,j}}] sU^n_{i,j} \qquad (5.87)$$

(b) Pumpage zone

$$-[\frac{KP_{x_{i-1/2,j}}}{\Delta x^2}] sP^*_{i-1,j} + \{[\frac{KP_{x_{i-1/2,j}}}{\Delta x^2}] + [\frac{KP_{x_{i+1/2,j}}}{\Delta x^2}]$$

$$+ \frac{2}{\Delta t} S_{oP_{i,j}}\} sP^*_{i,j} - [\frac{KP_{x_{i+1/2,j}}}{\Delta x^2}] sP^*_{i+1,j} = [\frac{KP_{y_{i,j-1/2}}}{\Delta x^2}] sP^n_{i,j-1}$$

$$- \{[\frac{KP_{y_{i,j-1/2}}}{\Delta x^2}] + [\frac{KP_{y_{i,j+1/2}}}{\Delta x^2}]\} sP^n_{i,j} + [\frac{KP_{x_{i,j+1/2}}}{\Delta x^2}] sP^n_{i,j+1}$$

$$+ \frac{2}{BP_{i,j}} \{KPU_{z_{i,j}} \frac{(sU^n_{i,j} - sP^n_{i,j})}{(BU_{i,j} + BP_{i,j})} - KLP_{z_{i,j}} \frac{(sP^n_{i,j} - sL^n_{i,j})}{(BP_{i,j} + BL_{i,j})}\}$$

$$+ \frac{Q_{i,j}}{\Delta x^2 BP_{i,j}} + [\frac{2}{\Delta t} S_{oP_{i,j}}] sP^n_{i,j} \qquad (5.88)$$

(c) Lower zone

$$-[\frac{KL_{x_{i-1/2}}}{\Delta x^2}] sL^*_{i-1,j} + \{[\frac{KL_{x_{i-1/2,j}}}{\Delta x^2}] + [\frac{KL_{x_{i+1/2,j}}}{\Delta x^2}]$$

$$+ \frac{2}{\Delta t} S_{oL_{i,j}}\} sL^*_{i,j} - [\frac{KL_{x_{i+1/2,j}}}{\Delta x^2}] sL^*_{i+1,j} = [\frac{KL_{y_{i,j-1/2}}}{\Delta x^2}] sL^n_{i,j-1}$$

$$- \{[\frac{KL_{y_{i,j-1/2}}}{\Delta x^2}] + [\frac{KL_{y_{i,j+1/2}}}{\Delta x^2}]\} sL^n_{i,j} + [\frac{KL_{x_{i,j+1/2}}}{\Delta x^2}] sL^n_{i,j+1}$$

$$+ \frac{2}{BL_{i,j}} \{KLP_{z_{i,j}} \frac{(sP^n_{i,j} - sL^n_{i,j})}{(BP_{i,j} + BL_{i,j})} - KLS_{z_{i,j}} \frac{(sL^n_{i,j} - sS^n_{i,j})}{(BL_{i,j} + BS_{i,j})}\}$$

$$+ \left[\frac{2}{\Delta t} S_{oL_{i,j}}\right] sP^{n}_{i,j} \tag{5.89}$$

(d) Saltwater zone

$$-\left[\frac{KS_{x_{i-1/2,j}}}{\Delta x^2}\right] sS^{*}_{i-1,j} + \left\{\left[\frac{KS_{x_{i-1/2,j}}}{\Delta x^2}\right] + \left[\frac{KS_{x_{i+1/2,j}}}{\Delta x^2}\right]\right.$$

$$\left. + \frac{2}{\Delta t} S_{oS_{i,j}}\right\} sS^{*}_{i,j} - \left[\frac{KS_{x_{i+1/2,j}}}{\Delta x^2}\right] sS^{*}_{i+1,j} = \left[\frac{KS_{x_{i,j-1/2}}}{\Delta x^2}\right] sS^{n}_{i,j-1}$$

$$- \left\{\left[\frac{KS_{x_{i,j-1/2}}}{\Delta x^2}\right] + \left[\frac{KS_{x_{i,j+1/2}}}{\Delta x^2}\right]\right\} sS^{n}_{i,j} + \left[\frac{KS_{x_{i,j+1/2}}}{\Delta x^2}\right] sS^{n}_{i,j+1}$$

$$+ \frac{2}{BS_{i,j}} \left\{KLS_{z_{i,j}} \frac{(sL^{n}_{i,j} - sS^{n}_{i,j})}{(BL_{i,j} + BS_{i,j})}\right\} + \left[\frac{2}{\Delta t} S_{oS_{i,j}}\right] sS^{n}_{i,j} \tag{5.90}$$

(2) Second iteration: computation in y direction

(a) Upper zone

$$-\left[\frac{KU_{y_{i,j-1/2}}}{\Delta x^2}\right] sU^{**}_{i,j-1} + \left\{\left[\frac{KU_{y_{i,j-1/2}}}{\Delta x^2}\right] + \left[\frac{KU_{y_{i,j+1/2}}}{\Delta x^2}\right]\right.$$

$$\left. + \frac{2}{\Delta t} S_{oU_{i,j}}\right\} sU^{**}_{i,j} - \left[\frac{KU_{y_{i,j+1/2}}}{\Delta x^2}\right] sU^{**}_{i,j+1} = -\left[\frac{KU_{y_{i,j-1/2}}}{\Delta x^2}\right] sU^{n}_{j-1}$$

$$+ \left\{\left[\frac{KU_{i,j-1/2}}{\Delta x^2}\right] + \left[\frac{KU_{i,j+1/2}}{\Delta x^2}\right]\right\} sU^{n}_{i,j}$$

$$- \left[\frac{KU_{y_{i,j+1/2}}}{\Delta x^2}\right] sU^{n}_{i,j+1} + \left[\frac{2}{\Delta t} S_{oU_{i,j}}\right] sU^{*}_{i,j} \tag{5.91}$$

(b) Pumpage zone

$$-\left[\frac{KP_{y_{i,j-1/2}}}{\Delta x^2}\right] sP^{**}_{i,j-1} + \left\{\left[\frac{KP_{y_{i,j-1/2}}}{\Delta x^2}\right] + \left[\frac{KP_{y_{i,j+1/2}}}{\Delta x^2}\right]\right.$$

$$\left. + \frac{2}{\Delta t} S_{oP_{i,j}}\right\} sP^{**}_{i,j} - \left[\frac{KP_{y_{i,j+1/2}}}{\Delta x^2}\right] sP^{**}_{i,j+1} = -\left[\frac{KP_{y_{i,j-1/2}}}{\Delta x^2}\right]$$

$$+ \{[\frac{KP\,y_{i,j-1/2}}{\Delta x^2}] + [\frac{KP\,x_{i,j+1/2}}{\Delta x^2}]\}sP^n_{i,j} + [\frac{KP\,y_{i,j+1/2}}{\Delta x^2}]sP^n_{i,j+1}$$

$$+ [\frac{2}{\Delta t}S_{oP_{i,j}}]sP^*_{i,j} \qquad (5.92)$$

(c) Lower zone

$$-[\frac{KL\,y_{i,j-1/2}}{\Delta x^2}]sl^{**}_{i,j-1} + \{[\frac{KL\,y_{i,j-1/2}}{\Delta x^2}] + [\frac{KL\,y_{i,j+1/2}}{\Delta x^2}]$$

$$+ \frac{2}{\Delta t}S_{oL_{i,j}}\}sL^{**}_{i,j} - [\frac{KL\,y_{i,j+1/2}}{\Delta x^2}]sL^{**}_{i,j+1} = -[\frac{KL\,y_{i,j-1/2}}{\Delta x^2}]sL^n_{i,j-1}$$

$$+ \{[\frac{KL\,y_{i,j-1/2}}{\Delta x^2}] + [\frac{KL\,y_{i,j+1/2}}{\Delta x^2}]\}sL^n_{i,j} - [\frac{KL\,y_{i,j+1/2}}{\Delta x^2}]sL^n_{i,j+1}$$

$$+ [\frac{2}{\Delta t}S_{oL_{i,j}}]sL^*_{i,j} \qquad (5.93)$$

(d) Saltwater zone

$$-[\frac{KS\,y_{i,j-1/2}}{\Delta x^2}]sS^{**}_{i,j-1} + \{[\frac{KS\,y_{i,j-1/2}}{\Delta x^2}] + [\frac{KS\,y_{i,j+1/2}}{\Delta x^2}]$$

$$+ \frac{2}{\Delta t}S_{oS_{i,j}}\}sS^{**}_{i,j} - [\frac{KS\,y_{i,j+1/2}}{\Delta x^2}]sS^{**}_{i,j+1} = -[\frac{KS\,y_{i,j+1/2}}{\Delta x^2}]sS^n_{i,j-1}$$

$$+ \{[\frac{KS\,y_{i,j-1/2}}{\Delta x^2}] + [\frac{KS\,y_{i,j+1/2}}{\Delta x^2}]\}sS^n_{i,j} - [\frac{KS\,y_{i,j+1/2}}{\Delta x^2}]sS^n_{i,j+1}$$

$$+ [\frac{2}{\Delta t}S_{oS_{i,j}}]sS^*_{i,j} \qquad (5.94)$$

(3) Third iteration: computation in z direction

(a) Upper zone

$$-[\frac{K'z_{i,j}}{DU_{i,j}}]\frac{(sH^{***}_{i,j} - sU^{***}_{i,j})}{B'_{i,j}} + \frac{2}{BU_{i,j}}KPU_{z_{i,j}}\frac{(sU^{***}_{i,j} - sP^{***}_{i,j})}{(BU_{i,j} + BP_{i,j})}$$

$$+ \left[\frac{2}{\Delta t} S_{oU_{i,j}}\right] sU^{***}_{i,j} = -\left[\frac{K'z_{i,j}}{BU_{i,j}}\right] \frac{(sH^{n}_{i,j} - sU^{n}_{i,j})}{B'_{i,j}}$$

$$+ \frac{2}{BU_{i,j}} KPU_{z_{i,j}} \frac{(sU^{n}_{i,j} - sP^{n}_{i,j})}{(BU_{i,j} + BP_{i,j})} + \left[\frac{2}{\Delta t} S_{oU_{i,j}}\right] sU^{**}_{i,j} \qquad (5.95)$$

(b) Pumpage zone

$$- \frac{2}{BP_{i,j}} \left\{ KPU_{z_{i,j}} \frac{(sU^{***}_{i,j} - sP^{***}_{i,j})}{(BU_{i,j} + BP_{i,j})} - KLP_{z_{i,j}} \frac{(sP^{***}_{i,j} - sL^{***}_{i,j})}{(BP_{i,j} + BL_{i,j})} \right\}$$

$$+ \left[\frac{2}{\Delta t} S_{oP_{i,j}}\right] sP^{***}_{i,j} = - \frac{2}{BP_{i,j}} \left\{ KPU_{z_{i,j}} \frac{(sU^{***}_{i,j} - sP^{***}_{i,j})}{(BU_{i,j} + BP_{i,j})} \right.$$

$$\left. - KLP_{z_{i,j}} \frac{(sP^{n}_{i,j} - sL^{n}_{i,j})}{(BP_{i,j} + BL_{i,j})} \right\} + \left[\frac{2}{\Delta t} S_{oP_{i,j}}\right] sP^{**}_{i,j} \qquad (5.96)$$

(c) Lower zone

$$- \frac{2}{BL_{i,j}} \left\{ KLP_{z_{i,j}} \frac{(sP^{***}_{i,j} - sL^{***}_{i,j})}{(BP_{i,j} + BL_{i,j})} - KLS_{z_{i,j}} \frac{(sL^{***}_{i,j} - sS^{***}_{i,j})}{(BL_{i,j} + BS_{i,j})} \right\}$$

$$+ \left[\frac{2}{\Delta t} S_{oL_{i,j}}\right] sL^{***}_{i,j} = - \frac{2}{BL_{i,j}} \left\{ KLP_{z_{i,j}} \frac{(sP^{n}_{i,j} - sL^{n}_{i,j})}{(BP_{i,j} + BL_{i,j})} \right.$$

$$\left. - KLS_{z_{i,j}} \frac{(sL^{n}_{i,j} - sS^{n}_{i,j})}{(BL_{i,j} + BS_{i,j})} \right\} + \left[\frac{2}{\Delta t} S_{oL_{i,j}}\right] sL^{**}_{i,j} \qquad (5.97)$$

(d) Saltwater zone

$$- \frac{2}{BS_{i,j}} \left\{ KLS_{z_{i,j}} \frac{(sL^{***}_{i,j} - sS^{***}_{i,j})}{(BL_{i,j} + BS_{i,j})} \right\} + \left[\frac{2}{\Delta t} S_{oS_{i,j}}\right] sS^{***}_{i,j}$$

$$= - \frac{2}{BS_{i,j}} \left\{ KLS_{z_{i,j}} \frac{(sL^{***}_{i,j} - sS^{***}_{i,j})}{(BL_{i,j} + BS_{i,j})} \right\} + \left[\frac{2}{\Delta t} S_{oS_{i,j}}\right] sS^{**}_{i,j} \qquad (5.98)$$

Equations 5.95 through 5.98 can be reduced to

$$(AA_1 + AA_2 + 2S_{oU_{i,j}}) sU^{***}_{i,j} - AA_2 sP^{***}_{i,j} = AA_8 \qquad (5.99a)$$

$$-(AA_3)sU^{***}_{i,j} + (AA_3 + AA_4 + 2S_{oP_{i,j}})sP^{***}_{i,j} - (AA_4)sL^{***}_{i,j} = AA_9 \quad (5.99b)$$

$$-(AA_5)sP^{***}_{i,j} + (AA_5 + AA_6 + 2S_{oL_{i,j}})sL^{***}_{i,j} - (AA_6)\,sS^{***}_{i,j} = AA_{10} \quad (5.99c)$$

$$-(AA_7)sL^{***}_{i,j} + (AA_7 + 2S_{oS_{i,j}})sS^{***}_{i,j} = AA_{11} \quad (5.99d)$$

where

$$AA_1 = \frac{K'_{z_{i,j}} \cdot \Delta t}{BU_{i,j} \cdot B_{i,j}} \quad (5.100)$$

$$AA_2 = \frac{2KPU_{z_{i,j}} \cdot \Delta t}{BU_{i,j}(BU_{i,j} + BP_{i,j})} \quad (5.101)$$

$$AA_3 = \frac{2KPU_{z_{i,j}} \cdot \Delta t}{BP_{i,j}(BU_{i,j} + BP_{i,j})} \quad (5.102)$$

$$AA_4 = \frac{2KLP_{z_{i,j}} \cdot \Delta t}{BP_{i,j}(BP_{i,j} + BL_{i,j})} \quad (5.103)$$

$$AA_5 = \frac{2KLP_{z_{i,j}} \cdot \Delta t}{BL_{i,j}(BP_{i,j} + BL_{i,j})} \quad (5.104)$$

$$AA_6 = \frac{2KLS_{z_{i,j}} \cdot \Delta t}{BL_{i,j}(BL_{i,j} + BS_{i,j})} \quad (5.105)$$

$$AA_7 = \frac{2KLS_{z_{i,j}} \cdot \Delta t}{BS_{i,j}(BL_{i,j} + BS_{i,j})} \quad (5.106)$$

$$AA_8 = AA_1(sH^{***}_{i,j} - sH^{n}_{i,j} + sU^{n}_{i,j}) + AA_2(sU^{n}_{i,j} - sP^{n}_{i,j}) + (2S_{oU_{i,j}})sU^{**}_{i,j} \quad (5.107)$$

$$AA_9 = AA_3(sP^{n}_{i,j} - sU^{n}_{i,j}) + AA_4(sP^{n}_{i,j} - sL^{n}_{i,j}) + (2S_{oP_{i,j}})sP^{**}_{i,j} \quad (5.108)$$

$$AA_{10} = AA_5(sL^n_{i,j} - sP^n_{i,j}) + AA_6(sL^n_{i,j} - sS^n_{i,j}) + (2S_{oL_{i,j}})sL^{**}_{i,j} \tag{5.109}$$

$$AA_{11} = AA_7(sS^n_{i,j} - sL^n_{i,j}) + (2S_{oS_{i,j}})sS^{**}_{i,j} \tag{5.110}$$

Equations 5.87 through 5.94 are solved using Thomas' algorithm (Benedict et al. 1983), a variant of Gauss' elimination algorithm. Since Equation 5.99 has only four unknowns ($sU^{***}_{i,j}$, $sP^{***}_{i,j}$, $sL^{***}_{i,j}$, and sS^{***},i,j; $sH^{***}_{i,j}$ is solved separately depending on the function of R, the net recharge to the water table), they are solved directly and an expression is derived for each of them as follows:

$$sP^{***}_{i,j} = \frac{AA_9 + \frac{(AA_3)(AA_8)}{AA_1 + AA_2 + 2S_{oU_{i,j}}} + \frac{(AA_4)}{(AA_{12})}\left[AA_{10} + \frac{(AA_6)(AA_7)}{AA_7 + 2S_{oS_{i,j}}}\right]}{AA_3 + AA_4 + 2S_{oP_{i,j}} - \frac{(AA_2)(AA_3)}{AA_1 + AA_2 + 2S_{oU_{i,j}}} - \frac{(AA_4)}{(AA_{12})}\left[AA_{10} + \frac{(AA_6)(AA_7)}{AA_7 + 2S_{oS_{i,j}}}\right]} \tag{5.111}$$

where

$$AA_{12} = AA_5 + AA_6 + 2S_{oL_{i,j}} - \frac{(AA_6)(AA_7)}{AA_7 + 2S_{oS_{i,j}}} \tag{5.112}$$

$$sU^{***}_{i,j} = \frac{AA_8 + (AA_2)sP^{***}_{i,j}}{AA_1 + AA_2 + 2S_{oU_{i,j}}} \tag{5.113}$$

$$sL^{***}_{i,j} = \frac{AA_{10} + \frac{(AA_6)(AA_7)}{AA_7 + 2S_{oS_{i,j}}} + (AA_5)sP^{**}_{i,j}}{AA_{12}} \tag{5.114}$$

$$sS^{***}_{i,j} = \frac{AA_{11} + (AA_7)sL^{***}_{i,j}}{AA_7 + 2S_{oS_{i,j}}} \tag{5.115}$$

The transport equations are solved in the following way:

(1) Determination of (ZDT)

(a) First iteration: computation in the x direction.

$$-[D_{xx_{i-\frac{1}{2},j}} - .25(D_{yx_{i,j+\frac{1}{2}}} - D_{yx_{i,j-\frac{1}{2}}})](ZDT)^{*}_{i-1,j}$$

$$+ \{D_{xx_{i-\frac{1}{2}}} + D_{xx_{i+\frac{1}{2}}} + \frac{2\Delta x^2}{\Delta t}[n - s_{o}L_{i,j}(sL^{n+\frac{1}{2}}_{i,j} - sL^{n}_{i,j})]\}(ZDT)^{*}_{i,j}$$

$$-[D_{xx_{i+\frac{1}{2}}} + .25(D_{yx_{i,j+\frac{1}{2}}} - D_{yx_{i,j-\frac{1}{2}}})](ZDT)^{*}_{i+1,j}$$

$$- \Delta x\{q^{L}_{x_{i-\frac{1}{2},j}}[{}^{(+)(ZDT)^{*}_{i-1,j}}_{(-)(ZDT)^{*}_{i,j}}] - q^{L}_{x_{i+\frac{1}{2}}}[{}^{(+)(ZDT)^{*}_{i,j}}_{(-)(ZDT)^{*}_{i+1,j}}]\}$$

$$= [D_{yy_{i,j-\frac{1}{2}}} - .25(D_{xy_{i+\frac{1}{2},j}} - D_{xy_{i-\frac{1}{2},j}})](ZDT)^{n}_{i,j-1}$$

$$- [D_{yy_{i,j-\frac{1}{2}}} + D_{yy_{i,j+\frac{1}{2}}}](ZDT)^{n}_{i,j} + [D_{yy_{i,j+\frac{1}{2}}}$$

$$+ .25(D_{xy_{i+\frac{1}{2},j}} - D_{xy_{i-\frac{1}{2}}})](ZDT)^{n}_{i,j+1} + \Delta x\{q^{L}_{i,j-\frac{1}{2}}[{}^{(+)(ZDT)^{n}_{i,j-1}}_{(-)(ZDT)^{n}_{i,j}}]$$

$$- q_{y_{i,j+\frac{1}{2}}}[{}^{(+)(ZDT)^{n}_{i,j}}_{(-)(ZDT)^{n}_{i,j+1}}]\} + .25\{D_{xy_{i+\frac{1}{2}}}[(ZDT)^{n}_{i+1,j+1}$$

$$- (ZDT)^{n}_{i+1,j-1}] - D_{xy_{i-\frac{1}{2},j}}[(ZDT)^{n}_{i-1,j+1} - (ZDT)^{n}_{i-1,j-1}]$$

$$+ D_{yx_{i,j+\frac{1}{2}}}[(ZDT)^{n}_{i+1,j+1} - (ZDT)^{n}_{i-1,j+1}] - D_{yx_{i,j+\frac{1}{2}}}[(ZDT)^{n}_{i+1,j-1}$$

$$- (ZDT)^{n}_{i-1,j-1}]\} - \Delta x(D_{xz_{i+\frac{1}{2},j}} - D_{xz_{i-\frac{1}{2},j}} + D_{yz_{i,j+\frac{1}{2}}}$$

$$- D_{yz_{i,j-\frac{1}{2}}}) + \Delta x^2 q_{z_o} \qquad (5.116)$$

(b) Second iteration: computation in the y direction

$$-[D_{yy_{i,j-\frac{1}{2}}} - .25(D_{xy_{i+\frac{1}{2},j}} - D_{xy_{i,-\frac{1}{2},j}})](ZDT)^{**}_{i,j-1}$$

$$+ \{D_{yy_{i,j-\frac{1}{2}}} + D_{yy_{i,j+\frac{1}{2}}} + \frac{2\Delta x^2}{\Delta t}[n - S_{oL_{i,j}}(sL^{n+\frac{1}{2}}_{i,j} - sL^{n}_{i,j})]\}(ZDT)^{***}_{i,j}$$

$$- [D_{yy_{i,j+\frac{1}{2}}} + .25(D_{xy_{i+\frac{1}{2},j}} - D_{xy_{i-\frac{1}{2},j}})](ZDT)^{**}_{i,j+1}$$

$$- \Delta x\{q^{L}_{y_{i,j-\frac{1}{2}}}[\begin{matrix}(+)(ZDT)^{**}_{i,j-1}\\(-)(ZDT)^{**}_{i,j}\end{matrix}] - a^{L}_{y_{i,j+\frac{1}{2}}}[\begin{matrix}(+)(ZDT)^{**}_{i,j}\\(-)(ZDT)^{**}_{i,j+1}\end{matrix}]$$

$$= -[D_{yy_{i,j-\frac{1}{2}}} - .25(D_{xy_{i+\frac{1}{2},j}} - D_{xy_{i-\frac{1}{2},j}})](ZDT)^{n}_{i,j-1}$$

$$+ [D_{yy_{i,j-\frac{1}{2}}} + D_{yy_{i,j+\frac{1}{2}}}](ZDT)^{n}_{i,j} = \frac{2\Delta x^2}{\Delta t}[n - S_{oL_{i,j}}(sL^{n+\frac{1}{2}}_{i,j}$$

$$- sL^{n}_{i,j})](ZDT)^{*}_{i,j} - [D_{yy_{i,j+\frac{1}{2}}} + .25(D_{xy_{i+\frac{1}{2},j}} - D_{xy_{i-\frac{1}{2},j}})](ZDT)^{n}_{i,j+1}$$

$$- \Delta x\{q^{L}_{y_{i,j-\frac{1}{2}}}[\begin{matrix}(+)(ZDT)^{n}_{i,j-1}\\(-)(ZDT)^{n}_{i,j}\end{matrix}] - q^{L}_{y_{i,j+\frac{1}{2}}}[\begin{matrix}(+)(ZDT)^{n}_{i,j}\\(-)(ZDT)^{n}_{i,j+1}\end{matrix}]\} \qquad (5.117)$$

(c) Third iteration: computation in the xy direction

$$(ZDT)^{***}_{i,j} = (ZDT)^{**}_{i,j} + \frac{.25}{\frac{2\Delta x^2}{\Delta t}[n - S_{oL_{i,j}}(sL^{n+\frac{1}{2}}_{i,j} - sL^{n}_{i,j})]}\{D_{xy_{i+\frac{1}{2}}}[(ZDT)^{**}_{i+1,j+1}$$

$$- (ZDT)^{n}_{i+1,j+1} - (ZDT)^{**}_{i+1,j-1} + (ZDT)^{n}_{i+1,j-1}] - D_{xy_{i-\frac{1}{2},j}}[(ZDT)^{**}_{i-1,j+1}$$

$$- (ZDT)^{n}_{i-1,j+1} - (ZDT)^{**}_{i-1,j-1} + (ZDT)^{n}_{i-1,j-1}] + D_{yx_{i,j+\frac{1}{2}}}[(ZDT)^{*}_{i+1,j+1}$$

$$- (ZDT)^{n}_{i+1,j+1} - (ZDT)^{*}_{i-1,j+1} + (ZDT)^{n}_{i-1,j+1}] - D_{yx_{i,j-\frac{1}{2}}}[(ZDT)^{*}_{i+1,j-1}$$

$$- (ZDT)^{n}_{i+1,j-1} - (ZDT)^{*}_{i-1,j-1} + (ZDT)^{n}_{i-1,j-1}]\} \qquad (5.118)$$

(2) Determination of Z_b and δ

(a) First estimate of Z_b: computation in x direction

$$- q^{L}_{x_{i-\frac{1}{2},j}}\left[\begin{matrix}(+)(Z^{*}_{b_{i-1,j}}) \\ (-)(0)\end{matrix}\right] + \frac{2\Delta x}{\Delta t}\left[n - S_{oL_{i,j}}(sL^{n+\frac{1}{2}}_{i,j} - sL^{n}_{i,j})\right] Z^{*}_{b_{i,j}}$$

$$-q^{L}_{x_{i-\frac{1}{2},j}}\left[\begin{matrix}(+)(0) \\ (-)(Z^{*}_{b_{i,j}})\end{matrix}\right] + q^{L}_{x_{i+\frac{1}{2},j}}\left[\begin{matrix}(+)(Z^{*}_{b_{i,j}}) \\ (-)(0)\end{matrix}\right] + q^{L}_{x_{i+\frac{1}{2},j}}\left[\begin{matrix}(+)(0) \\ (-)(Z_{b_{i+1,j}})\end{matrix}\right]$$

$$= \Delta x\, q_{z_{o_{i,j}}} - \frac{.5\, L'(0)}{\delta^{n}_{i,j}}\{D_{xz_{i+\frac{1}{2},j}}(Z^{n}_{b_{i+1,j}} - Z^{n}_{b_{i,j}})$$

$$+ D_{xz_{i-\frac{1}{2},j}}(Z^{n}_{b_{i,j}} - Z^{n}_{b_{i-1,j}}) + D_{yz_{i,j+\frac{1}{2}}}(Z^{n}_{b_{i,j+1}} - Z^{n}_{b_{i,j}})$$

$$+ D_{yz_{i,j-\frac{1}{2}}}(Z^{n}_{b_{i,j}} - Z^{n}_{b_{i,j-1}}) + 2\Delta x\, D_{zz_{i,j}}\} + q^{L}_{y_{i,j-\frac{1}{2}}}\left[\begin{matrix}(+)(Z^{n}_{b_{i,j-1}}) \\ (-)(Z^{n}_{b_{i,j}})\end{matrix}\right]$$

$$- q^{L}_{y_{i,j+\frac{1}{2}}}\left[\begin{matrix}(+)(Z^{n}_{b_{i,j}}) \\ (-)(Z^{n}_{b_{i,j+1}})\end{matrix}\right] + \frac{2\Delta x \cdot n}{\Delta t} Z^{n}_{b_{i,j}} \qquad (5.119)$$

(b) Second estimate of Z_b: computation in y direction

$$- q^L_{y_{i,j-1/2}} \begin{bmatrix} (+)(Z^{**}_{b_{i,j-1}}) \\ (-)(0) \end{bmatrix} + \frac{2\Delta x}{\Delta t} \left[n - S_{oL_{i,j}} (sL^{n+1/2}_{i,j} - sL^{n}_{i,j})\right] Z^{**}_{b_{i,j}}$$

$$- q^L_{y_{i,j-1/2}} \begin{bmatrix} (+)(0) \\ (-)(Z^{**}_{b_{i,j}}) \end{bmatrix} + q^L_{y_{i,j+1/2}} \begin{bmatrix} (+)(Z^{**}_{b_{i,j}}) \\ (-)(0) \end{bmatrix} + q^L_{y_{i,j+1/2}} \begin{bmatrix} (+)(0) \\ (-)(Z^{**}_{b_{i,j+1}}) \end{bmatrix}$$

$$= - q^L_{y_{i,j-1/2}} \begin{bmatrix} (+)(Z^{n}_{i,j-1}) \\ (-)(Z^{n}_{i,j}) \end{bmatrix} + q^L_{y_{i,j+1/2}} \begin{bmatrix} (+)(Z^{n}_{b_{i,j}}) \\ (-)(Z_{b_{i,j+1}}) \end{bmatrix}$$

$$+ \frac{2\Delta x}{\Delta t} \left[n - S_{oL_{i,j}} (sL^{n+1/2}_{i,j} - sL^{n}_{i,j})\right] Z^{*}_{b_{i,j}} \qquad (5.120)$$

(c) First estimate of δ: computation in xy direction

$$\delta^{**}_{i,j} = (ZDT^{***}_{i,j} - Z^{**}_{b_{i,j}}) / \left(\int_0^1 L(n)dn\right) \qquad (5.121)$$

(d) Final estimate of Z_b

$$Z^{***}_{b_{i,j}} = Z^{**}_{b_{i,j}} - \frac{.5\ L'(0)}{\delta^{**}_{i,j}} \{D_{xz_{i+1/2,j}} (Z^{**}_{b_{i,j+1}} - Z^{n}_{b_{i,j+1}} - Z^{**}_{b_{i,j}} + Z^{n}_{b_{i,j}})$$

$$+ D_{xz_{i-1/2,j}} (Z^{**}_{b_{i,j}} - Z^{n}_{b_{i,j}} - Z^{**}_{b_{i,j-1}} + Z^{n}_{b_{i,j-1}}) + D_{yz_{i,j+1/2}} (Z^{*}_{b_{i+1,j}}$$

$$- Z^{n}_{b_{i+1,j}} - Z^{*}_{b_{i,j}} + Z^{n}_{b_{i,j}}) + D_{yz_{i,j-1/2}} (Z^{*}_{b_{i,j}} - Z^{n}_{b_{i,j}} - Z^{*}_{b_{i-1,j}}$$

$$+ Z^{n}_{b_{i-1,j}})\} / \{\frac{2\Delta x}{\Delta t} \left[n - S_{oL_{i,j}} (sL^{n+1/2}_{i,j} - sL^{n}_{i,j})\right]\} \qquad (5.122)$$

(e) Final estimate of δ

$$\delta^{***}_{i,j} = (ZDT^{***}_{i,j} - Z^{***}_{b_{i,j}}) / \left(\int_0^1 L(n)dn\right) \qquad (5.123)$$

(3) Determination of ZDP

(a) If $(Z_{b_{i,j}} + \delta_{i,j}) < BL_{i,j}$

$$(ZDP)_{i,j} = 0 \tag{5.124a}$$

(b) If $Z_{b_{i,j}} < BL_{i,j} < (Z_{b_{i,j}} + \delta_{i,j})$

$$(ZDP)_{i,j} = 2\{[\delta\int_{n_L}^{1} L(n)dn]^{n+\frac{1}{2}} - [\delta\int_{n_L}^{1} L(n)dn]^{n}\}_{i,j}/\Delta t \tag{5.124b}$$

(c) If $Z_{b_{i,j}} > BL_{i,j}$

$$(ZDP)_{i,j} = 2[(ZDT)_{i,j}^{n+\frac{1}{2}} - (ZDT)_{i,j}^{n}]\ /\Delta t \tag{5.124c}$$

(4) Determination of $\frac{c}{c_s}$ in the pumpage zone

(a) First estimate of $\frac{c}{c_s}$: computation in x direction

$$\{\frac{2\Delta x}{\Delta t}[n - S_{oP_{i,j}}(sP_{i,j}^{n+\frac{1}{2}} - sP_{i,j}^{n})] + \frac{Q_{P_{i,j}}}{\Delta x \cdot BP_{i,j}}\}(\frac{c}{c_s})^{**}_{i,j}$$

$$- q^{P}_{y_{i,j-\frac{1}{2}}}\left[\frac{(+)(\frac{c}{c_s})^{**}_{i,j-1}}{(-)(\frac{c}{c_s})^{**}_{i,j}}\right] + q^{P}_{y_{i,j+\frac{1}{2}}}\left[\frac{(+)(\frac{c}{c_s})^{**}_{i,j}}{(-)(\frac{c}{c_s})^{**}_{i,j+1}}\right]$$

$$= q^{P}_{y_{i,j-\frac{1}{2}}}\left[\frac{(+)(\frac{c}{c_s})^{n}_{i,j-1}}{(-)(\frac{c}{c_s})^{n}_{i,j}}\right] - q^{P}_{y_{i,j+\frac{1}{2}}}\left[\frac{(+)(\frac{c}{c_s})^{n}_{i,j}}{(-)(\frac{c}{c_s})^{n}_{i,j-1}}\right] + \frac{(ZDP)_{i,j}}{BP_{i,j}} \tag{5.125}$$

(b) Second estimate of $\frac{c}{c_s}$: computation in y direction

$$\{\frac{2\Delta x}{\Delta t}[n - S_{oP_{i,j}}(sp^{n+\frac{1}{2}}_{i,j} - sp^{n}_{i,j})] + \frac{Q_{P_{i,j}}}{\Delta x \cdot BP_{i,j}}\}(\frac{c}{c_s})^{**}_{i,j}$$

$$- q^{P}_{y_{i,j-\frac{1}{2}}}\begin{bmatrix}(+)(\frac{c}{c_s})^{**}_{i,j-1}\\(-)(\frac{c}{c_s})^{**}_{i,j}\end{bmatrix} + q^{P}_{y_{i,j+\frac{1}{2}}}\begin{bmatrix}(+)(\frac{c}{c_s})^{**}_{i,j}\\(-)(\frac{c}{c_s})^{**}_{i,j+1}\end{bmatrix}$$

$$= -q^{P}_{y_{i,j-\frac{1}{2}}}\begin{bmatrix}(+)(\frac{c}{c_s})^{**}_{i,j-1}\\(-)(\frac{c}{c_s})^{n}_{i,j}\end{bmatrix} + a^{P}_{y_{i,j+\frac{1}{2}}}\begin{bmatrix}(+)(\frac{c}{c_s})^{n}_{i,j}\\(-)(\frac{c}{c_s})^{n}_{i,j+1}\end{bmatrix}$$

$$+ \{\frac{2\Delta x}{\Delta t}[n - S_{oP_{i,j}}(sp^{n+\frac{1}{2}}_{i,j} - sp^{n}_{i,j}) + \frac{Q_{P_{i,j}}}{\Delta x \cdot BP_{i,j}}\}(\frac{c}{c_s})^{*}_{i,j} \qquad (5.126)$$

The numerical model developed in the present chapter is a mathematical representation of the conceptual model of the aquifer system represented in Figure 4.2. Figure 5.5 shows the flow-chart of the computer code. It is common practice to use a model designed for a specific problem to study a different problem, with some simplifications and assumptions. On the other hand, the conceptual model is already a simplification of the real system. Since the mathematical model primarily deals with parameters (the aquifer's characteristics), the effects of the simplification and assumptions are generally reflected in those parameters. The analysis of the performance of the model including the sensitivity analysis of the solution variables to the input variables is carried on in the next chapter and shows the reliability of the model.

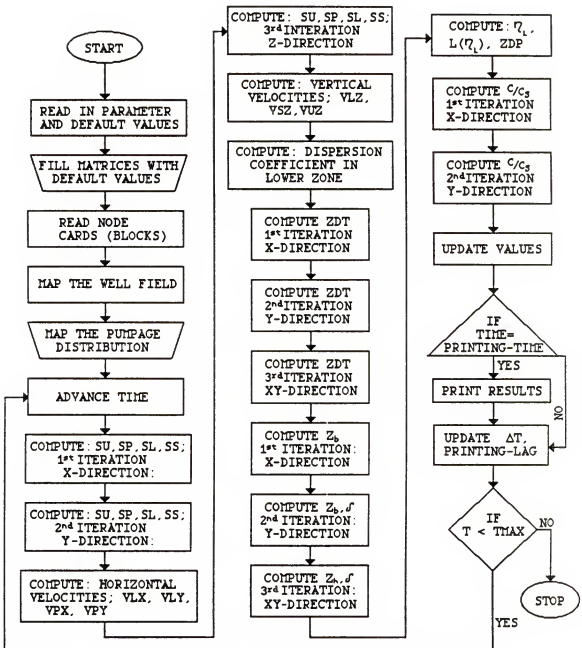

START
READ IN PARAMETER AND DEFAULT VALUES
FILL MATRICES WITH DEFAULT VALUES
READ NODE CARDS (BLOCKS)
MAP THE WELL FIELD
MAP THE PUMPAGE DISTRIBUTION
ADVANCE TIME
COMPUTE: SU, SP, SL, SS; 1st ITERATION X-DIRECTION:
COMPUTE: SU, SP, SL, SS; 2nd ITERATION Y-DIRECTION:
COMPUTE: HORIZONTAL VELOCITIES; VLX, VLY, VPX, VPY
COMPUTE: SU, SP, SL, SS; 3rd INTERATION Z-DIRECTION
COMPUTE: VERTICAL VELOCITIES; VLZ, VSZ, VUZ
COMPUTE: DISPERSION COEFFICIENT IN LOWER ZONE
COMPUTE ZDT 1st ITERATION X-DIRECTION
COMPUTE ZDT 2nd ITERATION Y-DIRECTION
COMPUTE ZDT 3rd ITERATION XY-DIRECTION
COMPUTE Zb 1st ITERATION: X-DIRECTION
COMPUTE Zb, d 2nd ITERATION: Y-DIRECTION
COMPUTE Zb, d 3rd ITERATION: XY-DIRECTION
COMPUTE: ηL, L(ηL), ZDP
COMPUTE C/Cs 1st ITERATION X-DIRECTION
COMPUTE C/Cs 2nd ITERATION Y-DIRECTION
UPDATE VALUES
IF TIME= PRINTING-TIME
YES
NO
PRINT RESULTS
UPDATE ΔT, PRINTING-LAG
IF T < TMAX
NO
YES
STOP

Figure 5.5 Flow Chart for the Upconing Simulation Program

CHAPTER 6
ANALYSIS OF THE PERFORMANCE OF THE MODEL

6.1 Introduction

The combination of numerical methods and digital computers has created a tool of immense power in the analysis of groundwater related problems. The practical question to be asked, while developing a numerical model to simulate a groundwater system, is how much one is willing to pay to obtain an answer to the considered problem. How closely the numerical model can approximate the real physical problem strongly depends on the answer to that question. Nevertheless, no complex physical problem such as a groundwater system, can be exactly reproduced by a numerical model; on the other hand, there is no error-free numerical model. The following analysis attempts to delineate the performance of the model described in the previous chapter.

One of the most vital and yet most difficult tasks of the development of a numerical model is the verification of the model. First, it must be established that the computer program is working as expected. It also must be established that the numerical solution of the problem is correct. Since the correct solution to the problem is not known beforehand, the approach commonly used is to simulate some limiting cases of the problem for which known solutions are available. However, because most existing solutions are based on assumptions that might differ from those used in the design of the numerical solution, the verification of a numerical model becomes a very complex and time

consuming task. For instance, the present model considers a confined aquifer of limited areal extent while the well-known Hantush analytical solution (Hantush, 1961) of drawdowns caused by a well partially penetrating a confined aquifer, considers an aquifer of infinite areal extent; yet the Hantush analytical solution will be used to verify the computation of the three-dimensional drawdown distribution by the numerical model. Models designed for practical purposes like the one in the present work, are generally verified using field data; but the problem with that approach is the lack of appropriate field data and the uncertainty related to those data. Except in a specific program designed to collect field data, the aquifer's parameters are not routinely measured. Variables such as transmissivities are generally obtained through pumping tests; even there, values generally obtained depend on the method of investigation used and on the mathematical model used in the analysis of the resulting test-data. The determination of an aquifer's characteristic parameters known as the "inverse problem" has been intensively discussed in groundwater literature (Todd, 1960; Bouwer, 1978; and Bear, 1979); Bear, 1979, wrote

> The selection of the appropriate formula is, perhaps, the most difficult part of a pumping test. . . . No methodology is available for selecting the most appropriate formula in a systematic way.
>
> (Bear, 1979, p. 466)

This statement applies to the determination of almost all the physical parameters which define an aquifer system. The general practice in the use of numerical models designed to simulate an aquifer system is the process known as the "calibration of the model."

In the present chapter, a sensitivity analysis has been conducted in order to determine the parameters which most influence the solution variables (i.e., the drawdowns, the rise of the saltwater front, the transition zone thickness, and the chloride concentration in water from the pumping well). The analytical solution of partially penetrating wells in a confined aquifer (Hantush, 1961) has been used in the verification of the drawdown obtained numerically. The analytical solution suggested by Bear and Dagan (1968) for the saltwater upconing (sharp interface theory) is used in the verification of the rise of the saltwater front under a single well. Finally, the model is applied to the simulation of the Titusville (Brevard County, Florida) wellfield.

6.2 Sensitivity Analysis of the Solution Variables to the Input Parameters

The analysis of any engineering problem should include a kind of error-analysis in the discussion of the results. The sensitivity analysis as performed here is one way the error-analysis of the numerical solutions can be carried out. On the other hand, in order to use the model effectively, the user needs to know what factors most influence the solution variables; another purpose of the sensitivity analysis is to show those influence factors. Finally, in the calibration process, the user needs to know how the solution variables vary with the influence factors, and the sensitivity analysis also gives hints on that aspect.

The main difference between the model developed in the present study and the existing solution models of the upconing problem is the consideration of the transition zone between the saltwater and the freshwater under the well. The parameters which *a priori* define the

importance of the mechanical dispersion and consequently that of the transition zone are the longitudinal and transversal dispersivities a_L and a_T. These parameters depend on the aquifer's physical constituents, and their values are almost nonexistent in the groundwater literature. Benedict et al. (1983) use $a_L = a_T = 0.5$m for Northeastern Florida; Segol and Pinder (1976) suggested $a_L = 6.667$ m and $a_T = 0.6667$ m for the Biscayne aquifer (Southeastern Florida). Both sets of values are considered in the present analysis. The case simulated here is well #19 in the Titusville wellfield; the pumping rate at the well is 374,700 gpd; the screened portion of the well measures 123 feet; the observed drawdown at the well is 44.5 feet while the observed concentration is over 1000 ppm. The history of the contamination is not known, and for the purpose of the simulation, it has been assumed that the chloride content in the well is over 1000 ppm after 4 years of pumping at a constant rate. Segol and Pinder's set of dispersivities has been used to calibrate the model and to obtain the value of the other parameters. Therefore, a comparison of the two "basic simulations" presented is not the purpose of the present analysis; only the influence of each parameter on the solution variables is sought. Table 6.1 gives the values of the input parameters for the two basic simulations using each set of dispersivity values.

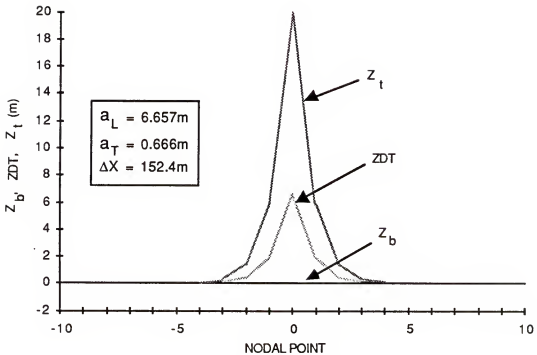
Figures 6.1 through 6.3 show the shape of the transition zone and that of the saltwater front, Z_b. The variable ZDT has been defined as

$$ZDT = Z_b + \delta \int_0^1 L(n)dn$$

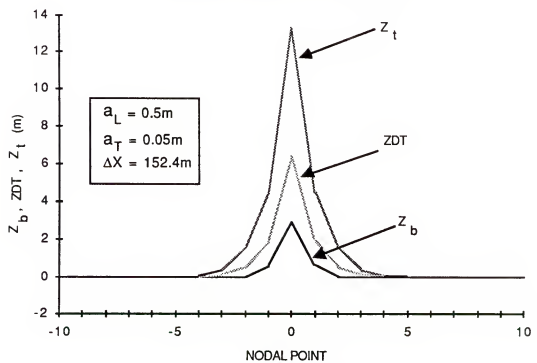
and represents the thickness that the saltwater mound would have if the chloride distribution in the transition zone was the same as that in the

Table 6.1 Parameter Values for the Basic Simulations

	Parameter's Description	Value
B'	Thickness of the semi-confining layer	0.91 m
BU	Thickness of the upper zone	3.05 m
BP	Thickness of the pumpage zone	37.49 m
BL	Thickness of the lower zone	26.15 m
BS	Thickness of the saltwater zone	15.55 m
K_h	Horizontal hydraulic conductivity	0.993 m/day
K_z	Vertical hydraulic conductivity	0.042 m/day
K'_z	Vertical hydraulic conductivity in the semi-confining layer	$4.084\ (10^{-5})$ m/day
S_o	Specific storage coefficient	$3.281\ (10^{-6})\ m^{-1}$
a_L	Longitudinal dispersivity (Case A)	6.657 m
	(Case B)	0.5 m
a_T	Transversal dispersivity (Case A)	0.666 m
	(Case B)	0.05 m
n	Effective porosity	0.30
ξ	Density ratio factor	0.025
Dx	Horizontal grid size	152.40 m

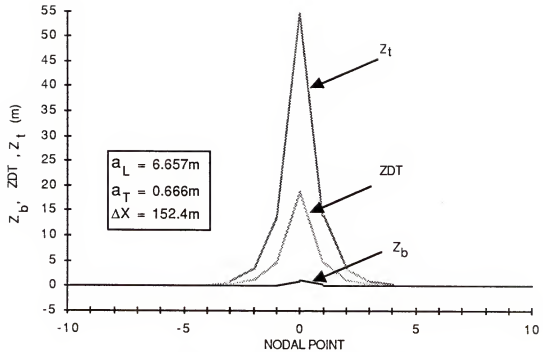


a. a_L = 6.657 m; a_T = 0.666 m

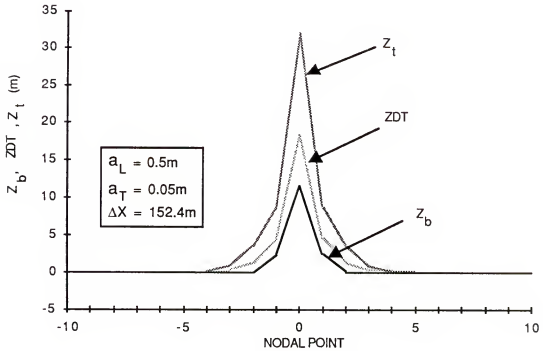


b. a_L = 0.5 m; a_T = 0.05 m

Figure 6.1 Shape of the Transition Zone and the Saltwater Front (T = 2 Years)

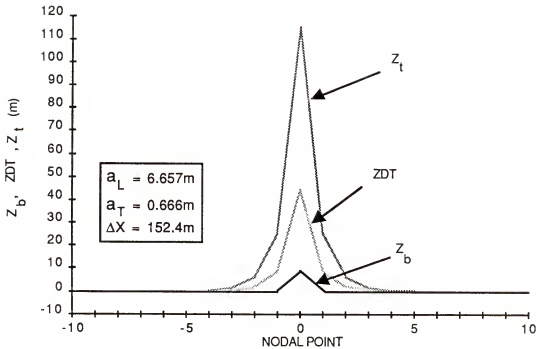


a. a_L = 6.657 m; a_T = 0.666 m

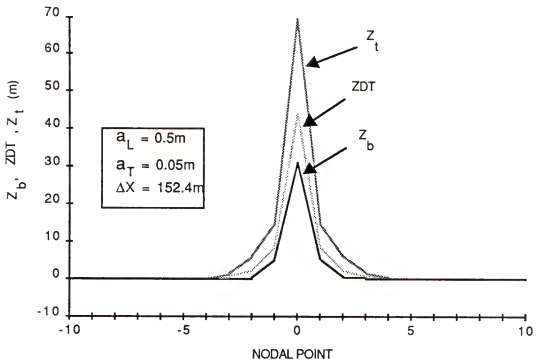


b. a_L = 0.5 m; a_T = 0.05 m

Figure 6.2 Shape of the Transition Zone and the Saltwater Front (T = 5 Years)



a. a_L = 6.657 m; a_T = 0.666 m



b. a_L = 0.5 m; a_T = 0.05 m

Figure 6.3 Shape of the Transition Zone and the Saltwater Front (T = 10 Years)

saltwater. In other words, if the saltwater mixed with the freshwater to form the transition zone could be separated, the thickness of the total saltwater above the initial position of the saltwater front, Z_o, would be equal to ZDT. The numerical value of the term $\int_0^1 L(n)dn$ being 1/3, when Z_b is zero as in the case shown in Figure 6.1a, ZDT equals $Z_t/3$; in that case, when ZDT equals BL/3, the top of the transition zone, Z_t, reaches the pumpage zone. It should be mentioned that the studies on the upconing phenomenon with the "sharp interface theory" also suggests that the rise of the saltwater front, Z_b, should be less than BL/3 to avoid the contamination of the well.

Figure 6.4 shows the time-concentration curves for the two basic simulations. The results from both cases show that the slopes of the concentration versus time curves decrease with time; this suggests that the concentration has a maximum value which will not be exceeded. The fact that the two curves mingle after a certain time (17 years from the figure) suggests that a factor other than the dispersivities controls the long term contamination. It can be shown that that factor is the vertical hydraulic conductivity which mainly controls the vertical flow.

The following analysis considers two cases: Case A: simulation using a_L = 6.667 m; and a_T = 0.6667 m; Case B: simulation using a_L = 0.5 m, and a_T = 0.05 m; and studies the sensitivity of the solution variables to the input variables. The solution variables are as follows:

sU= drawdown in the upper layer; (L)

sP= drawdown in the pumpage layer; (L)

sL= drawdown in the lower layer; (L)

sS= drawdown in the saltwater layer; (L)

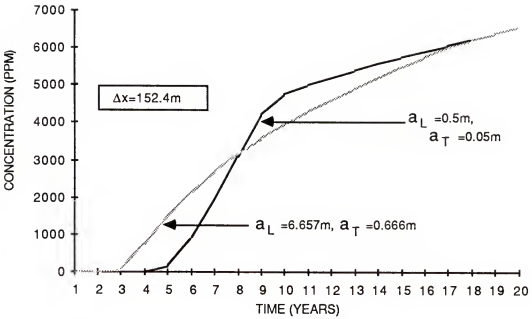


Figure 6.4 Time-Concentration Curves

ZDT= equivalent saltwater mound thickness; (L)

Z_b= elevation of the saltwater front; (L)

δ = thickness of the transition zone; (L)

Z_t= elevation of the top of the transition zone; (L)

C= chloride concentration in the pumpage zone; (PPM).

For each case of the basic simulations, each of the parameters in Table 6.1 has been modified with ±25% changes while all the others are kept constant. For instance the basic value of K_h is 0.993 m/day; thus, (K_h - 25%) and (K_h + 25%) are, respectively, 0.745 m/day and 1.241 m/day. The effects of those changes, considering the well-node as the point of interest, are shown in Tables 6.2 through 6.25. The analysis of those results shows that the well contamination process strongly depends on the dispersivity. Therefore, the sharp interface theory should be excluded from the study of saltwater upconing under a well in coastal aquifers underlain by saltwater.

A glance at Tables 6.2 through 6.25 indicates that the factors which significantly influence the drawdown distribution are the horizontal hydraulic conductivity K_y, the thickness of the pumpage zone BP, and the vertical hydraulic conductivity K_z. The factors which predominantly influence the chloride movement into the pumpage zone are the thickness of the pumpage zone BP, the thickness of the lower layer BL, the horizontal and vertical hydraulic conductivity K_h and K_z, the thickness of the saltwater zone BS, and the longitudinal dispersivity a_L. The influence of the grid size Δx is relative because of the theory of averaged values used in the development of the numerical model. According to the results in Table 6.14, the chloride content increases when Δx is reduced. However, using the basic finite-difference block of

Table 6.2 Sensitivity of sU to the Input Variables After 5-Year Simulation

The value from the basic simulation is: 12.440 m; (Cases A and B)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		sU (m)	Change in sU%	sU (m)	Change in sU%
BM	0.91 m	12.134	-2.460	12.640	+1.60
BU	3.05 m	12.893	+3.641	12.022	-3.360
BP	37.49 m	14.856	+19.421	10.656	-14.341
BL	26.15 m	12.688	+1.994	12.262	-1.431
BS	15.55 m	12.613	+1.391	12.290	-1.206
K_H	0.993 m/day	16.141	+29.751	10.101	-18.802
K_z	0.042 m/day	12.398	-0.338	12.410	-0.241
K'_z	$4.084(10^{-5})$m/day	12.693	+2.034	12.207	-1.873
S_o	$1.00(10^{-6})m^{-1}$	12.441	+0.008	12.440	0.00
A_L	6.657 m	12.440	0.00	12.440	0.00
A_T	0.666 m	12.440	0.00	12.440	0.00
Δx	152.40 m	12.783	+2.757	11.879	-4.510

Table 6.3 Sensitivity of sP to the Input Variables After 5-Year Simulation

The value from the basic simulation is: 14.173 m; (Cases A and B)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		sP (m)	Change in sP%	sP (m)	Change in sP%
BM	0.91 m	13.936	-1.672	14.330	1.108
BU	3.05 m	14.313	+0.988	14.044	-0.910
BP	37.49 m	16.538	+16.687	12.400	-12.510
BL	26.15 m	14.423	+1.764	13.998	-1.235
BS	15.55 m	14.353	+1.270	14.018	-1.094
K_H	0.993 m/day	17.967	+26.769	11.758	-17.039
K_z	0.042 m/day	14.646	+3.337	13.812	-2.547
K'_z	$4.084(10^{-5})$m/day	14.372	+1.404	13.992	-1.277
S_o	$1.00(10^{-6})m^{-1}$	14.174	+0.007	14.173	0.000
A_L	6.657 m	14.173	+0.000	14.173	0.000
A_T	0.666 m	14.173	+0.000	14.173	0.000
Δx	152.40 m	15.498	+9.349	13.079	-7.719

Table 6.4 Sensitivity of sL to the Input Variables After 5-Year Simulation

The value from the basic simulation is: 6.807 m; (Cases A and B)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		sL (m)	Change in sL%	sL (m)	Change in sL%
BM	0.91 m	6.604	-2.982	6.942	+1.983
BU	3.05 m	6.869	+0.911	6.747	-0.881
BP	37.49 m	8.156	+19.818	5.814	-14.588
BL	26.15 m	7.720	+13.413	6.069	-10.842
BS	15.55 m	7.063	+3.761	6.596	-3.100
K_H	0.993 m/day	9.343	+37.256	5.294	-22.277
K_z	0.042 m/day	6.390	-6.126	7.123	+4.642
K'_z	$4.084(10^{-5})$m/day	6.979	+2.527	6.652	-2.277
S_o	$1.00(10^{-6})m^{-1}$	6.808	+0.015	6.807	0.000
A_L	6.657 m	6.807	0.000	6.807	0.000
A_T	0.666 m	6.807	0.000	6.807	0.000
Δx	152.40 m	6.268	-7.918	7.093	+4.202

Table 6.5 Sensitivity of sS to the Input Variables After 5-Year Simulation

The value from the basic simulation is: 5.641 m; (Cases A and B)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		sS (m)	Change in sS%	sS (m)	Change in sS%
BM	0.91 m	5.445	-3.475	5.771	+2.305
BU	3.05 m	5.691	+0.886	5.592	-0.869
BP	37.49 m	6.625	+17.444	4.893	-13.260
BL	26.15 m	6.446	+14.271	5.000	-11.363
BS	15.55 m	6.126	+8.598	5.226	-7.357
K_H	0.993 m/day	7.879	+39.674	4.329	-23.258
K_z	0.042 m/day	5.181	-8.155	6.004	+6.435
K'_z	$4.084(10^{-5})$m/day	5.807	+2.943	5.491	-2.659
S_o	$1.00(10^{-6})m^{-1}$	5.642	0.018	5.641	0.00
A_L	6.657 m	5.641	0.00	5.641	0.00
A_T	0.666 m	5.641	0.00	5.641	0.00
Δx	152.40 m	5.019	-11.026	6.039	+7.055

Table 6.6 Sensitivity of ZDT to the Input Variables After 5-Year Simulation

The value from the basic simulation is: 18.877 m; (Case A)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		ZDT (m)	Change in ZDT%	ZDT (m)	Change in ZDT%
BM	0.91 m	18.695	-0.964	18.994	+0.620
BU	3.05 m	19.115	+1.261	18.658	-1.160
BP	37.49 m	25.533	+35.260	14.515	-23.107
BL	26.15 m	24.478	+29.671	14.915	-20.989
BS	15.55 m	16.526	-12.454	20.531	+8.762
K_H	0.993 m/day	23.225	+23.033	15.813	-16.231
K_z	0.042 m/day	14.862	-21.269	22.366	+18.483
K'_z	$4.084(10^{-5})$m/day	19.024	0.779	18.739	-0.731
S_o	$1.00(10^{-6})m^{-1}$	18.877	0.000	18.877	0.000
A_L	6.657 m	18.715	-0.858	19.037	+0.848
A_T	0.666 m	18.901	+0.127	18.852	-0.132
Δx	152.40 m	24.202	+28.209	15.390	-18.472

Table 6.7 Sensitivity of ZDT to the Input Variables After 5-Year Simulation

The value from the basic simulation is: 18.364 m; (Case B)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		ZDT (m)	Change in ZDT%	ZDT (m)	Change in ZDT%
BM	0.91 m	18.193	-0.931	18.474	+0.599
BU	3.05 m	18.599	+1.280	18.149	-1.171
BP	37.49 m	25.059	+36.457	14.028	-23.611
BL	26.15 m	23.991	+30.641	14.252	-22.392
BS	15.55 m	16.055	-12.574	19.981	+8.805
K_H	0.993 m/day	22.786	+24.080	15.275	-16.821
K_z	0.042 m/day	14.330	-21.967	21.898	+19.244
K'_z	$4.084(10^{-5})$m/day	18.502	+0.751	18.235	-0.702
S_o	$3.281(10^{-6})m^{-1}$	18.365	+0.005	18.364	0.000
A_L	0.5 m	18.352	-0.065	18.377	+0.071
A_T	0.05 m	18.366	+0.011	18.362	-0.011
Δx	152.40 m	23.085	+25.708	15.132	-17.600

Table 6.8 Sensitivity of Z_b to the Input Variables After 5-Year Simulation

The value from the basic simulation is: 1.030 m; (Case A)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		Z_b (m)	Change in Z_b%	Z_b (m)	Change in Z_b%
BM	0.91 m	0.987	-4.175	1.057	+2.621
BU	3.05 m	1.084	+5.243	0.980	-4.854
BP	37.49 m	2.784	+170.291	0.238	-76.893
BL	26.15 m	3.648	+254.175	0.036	-96.505
BS	15.55 m	0.326	-68.350	1.633	+58.544
K_H	0.993 m/day	2.565	+149.029	0.297	-71.165
K_z	0.042 m/day	0.151	-85.340	2.209	+114.466
K'_z	$4.084(10^{-5})$m/day	1.064	+3.301	0.998	-3.107
S_o	$1.00(10^{-6})m^{-1}$	1.030	0.000	1.030	0.000
A_L	6.657 m	2.091	+103.010	0.386	-62.524
A_T	0.666 m	1.037	+0.680	1.023	-0.680
Δx	152.40 m	1.515	+47.087	0.602	-41.553

Table 6.9 Sensitivity of Z_b to the Input Variables After 5-Year Simulation

The value from the basic simulation is: 11.559 m; (Case B)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		Z_b (m)	Change in Z_b%	Z_b (m)	Change in Z_b%
BM	0.91 m	11.427	-1.142	11.644	+0.735
BU	3.05 m	11.735	+1.523	11.398	-1.393
BP	37.49 m	16.546	+43.144	8.381	-27.494
BL	26.15 m	14.219	+23.012	7.110	-38.489
BS	15.55 m	9.405	-18.635	13.079	+13.150
K_H	0.993 m/day	15.197	+31.473	9.079	-21.455
K_z	0.042 m/day	8.336	-27.883	14.452	+25.028
K'_z	$4.084(10^{-5})$m/day	11.666	+0.926	11.459	-0.865
S_o	$3.281(10^{-6})m^{-1}$	11.559	0.000	11.559	0.000
A_L	0.5 m	12.215	+5.675	10.987	-4.949
A_T	0.05 m	11.736	+1.531	11.406	-1.324
Δx	152.40 m	14.586	+26.187	9.410	-18.592

Table 6.10 Sensitivity of δ to the Input Variables After 5-Year Simulation

The value from the basic simulation is: 53.541 m; (Case A)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		δ (m)	Change in δ%	δ (m)	Change in δ%
BM	0.91 m	53.123	-0.781	53.809	+0.501
BU	3.05 m	54.093	+1.031	53.032	-0.951
BP	37.49 m	68.247	+27.467	42.831	-20.003
BL	26.15 m	62.489	+16.712	44.637	-16.630
BS	15.55 m	48.602	-9.225	56.696	+5.893
K_H	0.993 m/day	61.978	+15.758	46.547	-13.063
K_z	0.042 m/day	44.134	-17.570	60.471	+12.943
K'_z	$4.084(10^{-5})$m/day	53.878	+0.629	53.224	-0.592
S_o	$1.00(10^{-6})m^{-1}$	53.542	+0.002	53.541	-0.000
A_L	6.657 m	49.873	-6.851	55.952	+4.503
A_T	0.666 m	53.594	+0.099	53.488	-0.099
Δx	152.40 m	68.062	+27.121	44.363	-17.142

Table 6.11 Sensitivity of δ to the Input Variables After 5-Year Simulation

The value from the basic simulation is: 20.416 m; (Case B)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		δ (m)	Change in δ%	δ (m)	Change in δ%
BM	0.91 m	20.298	-0.578	20.491	0.367
BU	3.05 m	20.594	+0.872	20.254	-0.793
BP	37.49 m	25.539	+25.093	16.941	-17.021
BL	26.15 m	29.315	+43.588	21.427	+4.952
BS	15.55 m	19.951	-2.278	20.704	+1.411
K_H	0.993 m/day	22.765	+11.506	18.588	-8.954
K_z	0.042 m/day	17.983	-11.917	22.338	+9.414
K'_z	$4.084(10^{-5})$m/day	20.510	+0.460	20.327	-0.436
S_o	$3.281(10^{-6})m^{-1}$	20.417	+0.005	20.416	0.000
A_L	0.5 m	18.412	-9.816	22.170	+8.591
A_T	0.05 m	19.890	-2.576	20.868	+2.214
Δx	152.40 m	25.498	+24.892	17.166	-15.919

Table 6.12 Sensitivity of Z_t to the Input Variables After 5-Year Simulation

The value from the basic simulation is: 54.571 m; (Case A)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		Z_t (m)	Change in Z_t%	Z_t (m)	Change in Z_t%
BM	0.91 m	54.110	-0.845	54.866	0.541
BU	3.05 m	55.178	+1.112	54.013	-1.023
BP	37.49 m	71.031	+30.163	43.070	-21.075
BL	26.15 m	66.137	+21.194	44.673	-18.138
BS	15.55 m	48.928	-10.341	58.329	+6.886
K_H	0.993 m/day	64.544	+18.275	46.844	-14.160
K_z	0.042 m/day	44.285	-18.849	62.680	+14.860
K'_z	$4.084(10^{-5})$m/day	54.943	+0.682	54.222	-0.640
S_o	$1.00(10^{-6})m^{-1}$	54.572	+0.002	54.571	0.000
A_L	6.657 m	51.964	-4.777	56.338	3.238
A_T	0.666 m	54.631	+0.110	54.511	-0.110
Δx	152.40 m	69.576	+27.496	44.965	-17.603

Table 6.13 Sensitivity of Z_t to the Input Variables After 5-Year Simulation

The value from the basic simulation is: 31.975 m; (Case B)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		Z_t (m)	Change in Z_t%	Z_t (m)	Change in Z_t%
BM	0.91 m	31.726	-0.779	32.135	+0.500
BU	3.05 m	32.329	+1.107	31.652	-1.010
BP	37.49 m	42.085	+31.618	25.322	-20.807
BL	26.15 m	43.534	+36.150	28.536	-10.755
BS	15.55 m	29.356	-8.191	33.783	+5.654
K_H	0.993 m/day	37.962	+18.724	27.667	-13.473
K_z	0.042 m/day	26.318	-17.692	36.790	+15.059
K'_z	$4.084(10^{-5})$m/day	32.176	+0.629	31.786	-0.591
S_o	$3.281(10^{-6})m^{-1}$	31.976	+0.003	31.975	0.000
A_L	0.5 m	30.625	-4.222	33.157	+3.697
A_T	0.05 m	31.626	-1.091	32.275	+0.938
Δx	152.40 m	40.084	+25.360	26.576	-16.885

Table 6.14 Sensitivity of C to the Input Variables After 5-Year Simulation

The value from the basic simulation is: 1510.036 ppm; (Case A)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		C (ppm)	Change in C%	C (ppm)	Change in C%
BM	0.91 m	1471.342	-2.562	1534.991	+1.653
BU	3.05 m	1559.358	+3.266	1464.855	-2.992
BP	37.49 m	3041.497	+101.419	599.168	-60.321
BL	26.15 m	3311.261	+119.284	284.851	-81.136
BS	15.55 m	1073.045	-28.939	1832.782	+21.373
K_H	0.993 m/day	2331.701	54.414	930.732	-38.364
K_Z	0.042 m/day	751.047	-50.263	2174.893	+44.029
K'_Z	$4.084(10^{-5})$m/day	1541.473	+2.082	1408.694	-1.943
S_o	$1.00(10^{-6})m^{-1}$	1510.114	+0.005	1510.003	-0.002
A_L	6.657 m	1347.478	-10.765	1645.271	+8.956
A_T	0.666 m	1514.878	+0.321	1505.150	-0.324
Δx	152.40 m	1763.094	+16.758	993.761	-34.190

Table 6.15 Sensitivity of C to the Input Variables After 5-Year Simulation

The value from the basic simulation is: 181.379 ppm; (Case B)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		C (ppm)	Change in C%	C (ppm)	Change in C%
BM	0.91 m	163.726	-9.733	193.189	+6.511
BU	3.05 m	207.793	+14.563	158.906	-12.390
BP	37.49 m	1755.571	+867.902	10.000	-
BL	26.15 m	3022.754	+1566.540	10.000	-
BS	15.55 m	43.898	-75.798	356.764	+96.695
K_H	0.993 m/day	910.778	+402.141	14.334	-92.097
K_Z	0.042 m/day	10.002	-94.486	723.382	+298.823
K'_Z	$4.084(10^{-5})$m/day	196.325	+8.240	167.923	-7.419
S_o	$3.281(10^{-6})m^{-1}$	181.421	+0.023	181.382	+0.002
A_L	0.5 m	112.594	-37.923	248.126	+36.800
A_T	0.05 m	162.298	-10.520	198.254	+9.304
Δx	152.40 m	813.042	+348.256	10.087	-94.439

Table 6.16 Sensitivity of ZDT to the Input Variables After 10-Year Simulation

The value from the basic simulation is: 44.449 m; (Case A)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		ZDT (m)	Change in ZDT%	ZDT (m)	Change in ZDT%
BM	0.91 m	43.921	-1.188	44.791	0.769
BU	3.05 m	45.051	+1.354	43.894	-1.249
BP	37.49 m	60.550	+36.224	33.784	-23.994
BL	26.15 m	57.501	+29.364	35.031	-21.188
BS	15.55 m	38.492	-13.402	48.797	+9.782
K_H	0.993 m/day	53.867	+21.188	37.566	-15.485
K_Z	0.042 m/day	35.312	-20.556	52.158	+17.343
K'_Z	$4.084(10^{-5})$m/day	44.879	+0.967	44.048	-0.902
S_O	$1.00(10^{-6})m^{-1}$	44.451	+0.004	44.449	0.000
A_L	6.657 m	44.238	-0.475	44.656	+0.466
A_T	0.666 m	44.509	+0.135	44.390	-0.133
Δx	152.40 m	61.655	+38.710	34.383	-22.646

Table 6.17 Sensitivity of ZDT to the Input Variables After 10-Year Simulation

The value from the basic simulation is: 43.872 m; (Case B)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		ZDT (m)	Change in ZDT%	ZDT (m)	Change in ZDT%
BM	0.91 m	43.361	-1.165	44.200	+0.748
BU	3.05 m	44.479	+1.384	43.312	-1.276
BP	37.49 m	60.452	+37.792	33.048	-24.672
BL	26.15 m	57.220	+30.425	33.932	-22.657
BS	15.55 m	37.955	-13.487	48.164	+9.783
K_H	0.993 m/day	53.644	22.274	36.799	-16.122
K_Z	0.042 m/day	34.520	-21.317	51.832	+18.144
K'_Z	$4.084(10^{-5})$m/day	44.286	+0.944	43.384	-0.884
S_O	$1.00(10^{-6})m^{-1}$	43.873	+0.002	43.872	0.000
A_L	0.5 m	43.854	-0.041	43.888	+0.036
A_T	0.05 m	43.876	+0.009	43.866	-0.014
Δx	152.40 m	60.481	+37.858	34.093	-22.290

Table 6.18 Sensitivity of Z_b to the Input Variables After 10-Year Simulation

The value from the basic simulation is: 9.002 m; (Case A)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		Z_b (m)	Change in Z_b%	Z_b (m)	Change in Z_b%
BM	0.91 m	8.824	-1.977	9.118	+1.289
BU	3.05 m	9.218	+2.399	8.804	-2.200
BP	37.49 m	15.112	+67.874	5.322	-40.880
BL	26.15 m	16.513	+83.437	4.334	-51.855
BS	15.55 m	6.180	-31.349	11.404	+26.683
K_H	0.993 m/day	13.930	+54.743	5.888	-34.592
K_z	0.042 m/day	5.004	-44.412	12.896	+43.257
K'_z	$4.084(10^{-5})$m/day	9.148	+1.622	8.867	-1.500
S_o	$1.00(10^{-6})m^{-1}$	9.003	+0.011	9.002	0.000
A_L	6.657 m	11.325	+25.805	7.148	-20.595
A_T	0.666 m	9.347	+3.832	8.889	-1.255
Δx	152.40 m	13.097	+45.490	6.893	-23.428

Table 6.19 Sensitivity of Z_b to the Input Variables After 10-Year Simulation

The value from the basic simulation is: 31.117 m; (Case B)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		Z_b (m)	Change in Z_b%	Z_b (m)	Change in Z_b%
BM	0.91 m	30.716	-1.289	31.375	+0.829
BU	3.05 m	31.589	+1.517	30.682	-1.398
BP	37.49 m	43.929	+41.174	22.812	-26.690
BL	26.15 m	32.450	+4.284	17.540	-43.632
BS	15.55 m	25.472	-18.141	35.259	+13.311
K_H	0.993 m/day	39.418	+26.677	25.235	-18.903
K_z	0.042 m/day	23.376	-24.877	37.832	+21.580
K'_z	$4.084(10^{-5})$m/day	31.443	+1.048	30.813	-0.977
S_o	$3.281(10^{-6})m^{-1}$	31.118	+0.003	31.116	-0.003
A_L	0.5 m	32.084	+3.108	30.258	-2.761
A_T	0.05 m	31.701	+1.877	30.613	-1.620
Δx	152.40 m	43.148	+38.664	23.978	-22.942

Table 6.20 Sensitivity of δ to the Input Variables After 10-Year Simulation

The value from the basic simulation is: 106.343 m; (Case A)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		δ (m)	Change in δ%	δ (m)	Change in δ%
BM	0.91 m	105.289	-0.991	107.020	0.637
BU	3.05 m	107.501	+1.089	105.270	-1.009
BP	37.49 m	136.316	+28.185	85.387	-19.706
BL	26.15 m	122.964	+15.630	92.091	-13.402
BS	15.55 m	96.934	-8.848	112.179	+5.488
K_H	0.993 m/day	119.811	+12.665	95.034	-10.634
K_z	0.042 m/day	90.924	-14.499	117.786	+10.760
K'_z	$4.084(10^{-5})$m/day	107.193	+0.799	105.544	-0.751
S_o	$1.00(10^{-6})m^{-1}$	106.345	+0.002	106.341	-0.002
A_L	6.657 m	98.738	-7.151	112.525	+5.813
A_T	0.666 m	105.484	-0.808	106.504	+0.151
Δx	152.400 m	145.673	+36.984	82.470	-22.449

Table 6.21 Sensitivity of δ to the Input Variables After 10-Year Simulation

The value from the basic simulation is: 38.265 m; (Case B)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		δ (m)	Change in δ%	δ (m)	Change in δ%
BM	0.91 m	37.934	-0.865	38.474	+0.546
BU	3.05 m	38.671	+1.061	37.890	-0.980
BP	37.49 m	49.570	+29.544	30.709	-19.747
BL	26.15 m	74.309	+94.196	49.177	+28.517
BS	15.55 m	37.451	-2.127	38.716	+1.179
K_H	0.993 m/day	42.680	+11.538	34.692	-9.338
K_z	0.042 m/day	33.433	-12.628	41.999	+9.758
K'_z	$4.084(10^{-5})$m/day	38.529	+0.690	38.014	-0.656
S_o	$3.281(10^{-6})m^{-1}$	38.266	+0.003	38.265	0.000
A_L	0.5 m	35.311	-7.720	40.890	+6.860
A_T	0.05 m	36.524	-4.550	39.759	+3.904
Δx	152.40 m	51.999	+35.892	30.346	-20.695

Table 6.22 Sensitivity of Z_t to the Input Variables After 10-Year Simulation

The value from the basic simulation is: 115.344 m; (Case A)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		Z_t (m)	Change in Z_t%	Z_t (m)	Change in Z_t%
BM	0.91 m	114.114	-1.066	116.138	+0.688
BU	3.05 m	116.719	+1.192	114.074	-1.101
BP	37.49 m	151.428	+31.284	90.709	-21.358
BL	26.15 m	139.477	+20.923	96.424	-16.403
BS	15.55 m	103.115	-10.602	123.583	+7.143
K_H	0.993 m/day	133.741	+15.950	100.922	-12.503
K_z	0.042 m/day	95.928	-16.833	130.682	+13.298
K'_z	$4.084(10^{-5})$m/day	116.341	+0.864	114.411	-0.809
S_o	$1.00(10^{-6})m^{-1}$	115.348	+0.003	115.343	-0.001
A_L	6.657 m	110.064	-4.578	119.673	+3.753
A_T	0.666 m	114.832	-0.444	115.392	+0.042
Δx	152.40 m	158.771	+37.650	89.363	-22.525

Table 6.23 Sensitivity of Z_t to the Input Variables After 10-Year Simulation

The value from the basic simulation is: 69.382 m; (Case B)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		Z_t (m)	Change in Z_t%	Z_t (m)	Change in Z_t%
BM	0.91 m	68.650	-1.055	69.850	0.675
BU	3.05 m	70.260	+1.265	68.572	-1.167
BP	37.49 m	93.499	+34.760	53.521	-22.860
BL	26.15 m	106.760	+53.873	66.716	-3.842
BS	15.55 m	62.922	-9.311	73.974	+6.618
K_H	0.993 m/day	82.098	+18.328	59.927	-13.627
K_z	0.042 m/day	56.809	-18.121	79.831	+15.060
K'_z	$4.084(10^{-5})$m/day	69.972	+0.850	68.827	-0.800
S_o	$3.281(10^{-6})m^{-1}$	69.383	+0.001	69.382	0.000
A_L	0.5 m	67.394	-2.865	71.148	+2.545
A_T	0.05 m	68.225	-1.668	70.373	+1.428
Δx	152.40 m	95.147	+37.135	54.324	-21.703

Table 6.24 Sensitivity of C to the Input Variables After 10-Year Simulation

The value from the basic simulation is: 3951.131 ppm; (Case A)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		C (ppm)	Change in C%	C (ppm)	Change in C%
BM	0.91 m	3876.137	-1.898	3999.884	+1.234
BU	3.05 m	4027.599	+1.935	3880.274	-1.793
BP	37.49 m	5989.374	+51.586	2597.606	-34.257
BL	26.15 m	6004.521	+51.970	2478.731	-37.265
BS	15.55 m	3196.161	-19.108	4519.573	+14.387
K_H	0.993 m/day	5006.732	+26.716	3173.128	-19.691
K_Z	0.042 m/day	2907.578	-26.412	4830.343	+22.252
K'_Z	$4.084(10^{-5})$m/day	4012.296	+1.548	3894.245	-1.440
S_o	$1.00(10^{-6})m^{-1}$	3951.345	+0.005	3951.008	-0.003
A_L	6.657 m	3962.527	+0.288	3955.209	+0.103
A_T	0.666 m	3936.775	-0.363	3955.696	+0.116
Δx	152.40 m	3910.164	-1.037	3818.322	-3.361

Table 6.25 Sensitivity of C to the Input Variables After 10-Year Simulation

The value from the basic simulation is: 4747.252 ppm; (Case B)

Input Parameters	Basic Value of the Input Parameter	-25% Change in the Basic Input Parameter		+25% Change in the Basic Input Parameter	
		C (ppm)	Change in C%	C (ppm)	Change in C%
BM	0.91 m	4670.466	-1.617	4796.153	+1.030
BU	3.05 m	4825.707	+1.653	4672.864	-1.567
BP	37.49 m	6670.791	+40.519	2550.028	-46.284
BL	26.15 m	6277.920	+32.243	2074.875	-56.293
BS	15.55 m	3658.739	-22.929	5307.183	+11.795
K_H	0.993 m/day	5738.046	+20.871	3546.243	-25.299
K_Z	0.042 m/day	3005.349	-36.693	5582.824	+17.601
K'_Z	$4.084(10^{-5})$m/day	4808.838	+1.297	4689.236	-1.222
S_o	$3.281(10^{-6})m^{-1}$	4747.476	+0.005	4747.243	-0.0002
A_L	0.5 m	4760.000	+0.269	4731.083	-0.341
A_T	0.05 m	4754.164	+0.146	4739.726	-0.159
Δx	152.40 m	4159.980	-12.371	4007.531	-15.582

horizontal grid size of (152.4 x 152.4) m^2, the average chloride content obtained at the well after 5 years of simulation is 1510.036 ppm. The volume of saltwater in the pumping cell (block containing the well) can be obtained as

$$Vol_{s1} = \frac{n \cdot BP \times (152.4)^2 \times 1510,036}{c_s}$$

Using a finite difference block of reduced horizontal grid size of [152.4 (1 - 0.25) x 152.4 (1 - 0.25)] m^2, the average chloride content obtained after 5 years of simulation is 1763.094 ppm and the volume of saltwater in the pumping cell is

$$Vol_{s2} = \frac{n \cdot BP \times [152.4\ (1 - 0.25)]^2 \times 1763.094}{c_s}$$

The relative change (%) in the saltwater volume is

$$\frac{\Delta\ Vol_s}{Vol_{s1}} = \frac{Vol_{s2} - Vol_{s1}}{Vol_{s1}} = -34.32\%$$

which suggests that the overall chloride induced in the pumpage zone decreases when Δx is reduced. The same analysis with 25% increase in Δx holds 2.829% increase in the volume of chloride induced in the pumping cell. This analysis considers the case where the transition zone reaches the well node only. If the transition zone has covered more than one node, the analysis could be done differently (see Figure 6.17). The effect of Δx in the pumping cell is also time dependent; as can be seen in Table 6.12, after 10-year simulation, that effect is reduced to an average change of 2.2%. Furthermore, the effect of neglecting the dispersion in the pumpage zone, to some extent, might be compensated by using large grid size Δx.

This analysis only shows the factors which significantly influence the solution variables for the example studied here. It does not give the degree of accuracy of the model. The comparison which follows shows how the numerical solutions compare with the existing solutions.

6.3 Verification of the Drawdown

The hydraulics of partially penetrating wells is different from that of wells that fully penetrate the aquifer. The problem of partial penetration of wells has long been recognized and many investigations on the topic have given several approximate solutions for various field conditions (Hantush 1961). However, the most commonly reported solution in groundwater literature is the Hantush solution which is used here for the verification of the numerical solution of the drawdown given by UPCON.

The drawdown, s, in a piezometer having a depth of penetration, z, and being at a distance, r, from a steadily discharging well that partially penetrates a confined aquifer of inifinite areal extent is given by (Hantush 1961).

$$s = \frac{Q}{4\pi Kb}\left[W(u) + f\left(u, \frac{r}{b}, \frac{\ell}{b}, \frac{d}{b}, \frac{z}{b}\right)\right] \qquad (6.1)$$

where

Q = well discharge (L^3T^{-1})

K = hydraulic conductivity (LT^{-1})

r = radial distance from the well (L)

$W(u)$ = standard well function (Theis' solution for non-leaky aquifers)

$$f = \frac{2b}{\pi(\ell-d)} \sum_{n=1}^{\alpha} \frac{1}{n}\left(\sin\frac{n\pi\ell}{b} - \sin\frac{n\pi d}{b}\right)\cos\frac{n\pi Z_p}{b}\, W\left(u, \frac{n\pi r}{b}\right) \qquad (6.2)$$

$$u = \frac{r^2 S_o}{4kt} \tag{6.3}$$

t = time since pumping started (T)

S_o = specific storage (L^{-1})

W(u,y) = well function for leaky aquifers

The remaining terms of Equations 6.1 and 6.2 are defined in Figure 6.5.

The average drawdown, $\bar{s}$, in an observation well screened between the depths d' and ℓ' (ℓ' > d') is given by (Hantush, 1961).

$$\bar{s} = \frac{Q}{4\pi Kb}\left[W(u) + \bar{f}\left(u, \frac{r}{b}, \frac{\ell}{b}, \frac{d}{b}, \frac{\ell'}{b}, \frac{d'}{b}\right)\right] \tag{6.4}$$

in which

$$\bar{f} = \frac{2b^2}{\pi^2(\ell-d)(\ell'-d')} \sum_{n=1}^{\infty} \frac{1}{n^2}\left(\sin\frac{n\pi\ell}{b} - \sin\frac{n\pi d}{b}\right)\left(\sin\frac{n\pi\ell'}{b} - \sin\frac{n\pi d'}{b}\right)W\left(u, \frac{n\pi r}{b}\right) \tag{6.5}$$

Equation 6.4 is obtained by integrating Equation 6.1 over the screened portion of the observation well.

In order to apply Equation 6.4 to the upconing problem, an imaginary observation well has been placed at each nodal point of each layer. Figure 6.6 shows the representation of the observation wells in each layer. Hantush (1961) suggests that the partial penetration of the well does not affect a point situated at a distance larger than 1.5b. The total thickness of the aquifer simulated in the present analysis has therefore been exaggerated in order to have an acceptable number of points of comparison. On the other hand, Equation 6.1 has been developed for an homogeneous and isotropic aquifer; therefore, the vertical and horizontal hydraulic conductivities are equal and constant

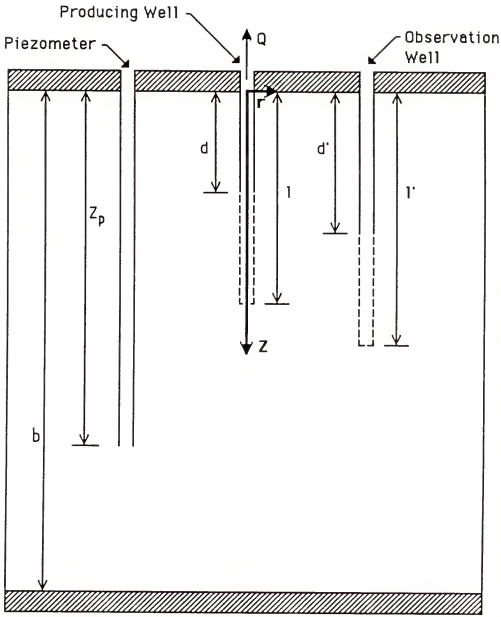


Figure 6.5 Conceptual Aquifer's Representation for Hantush's 3-D Drawdown Solution

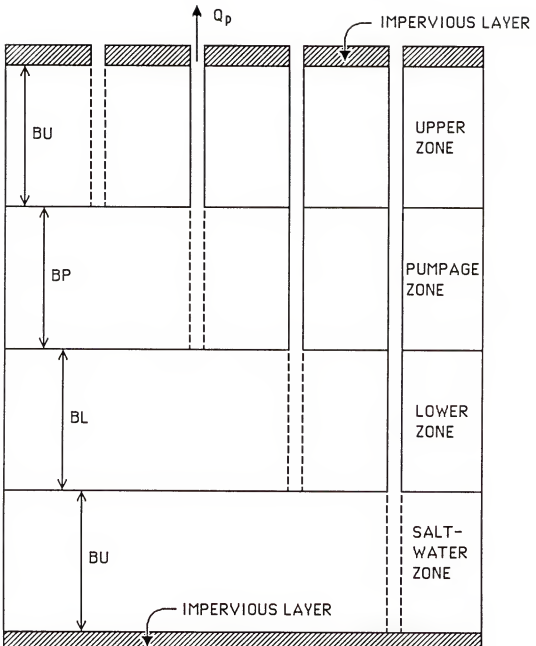


Figure 6.6 Conceptual Representation for the Verification of the Numerical and Hantush's Analytical Solutions for the Drawdowns

throughout the aquifer system. Table 6.26 gives the aquifer's characteristic values used in this analysis. Figure 6.7 shows the vertical distribution of the drawdown at the well node; the two curves are obtained using Equations 6.1 and 6.5. It is evident from the figure that Equation 6.5 effectively gives the vertically averaged drawdown in each layer. Figure 6.8 shows the analytical and numerical solution of the drawdown distribution along the x axis, in the pumpage and in the lower zone. The difference in the two solutions at the well itself can be explained by the approach used in each method: the analytical solution represents the well by a line sink, while the numerical solution considers a finite-difference block as representing the well. Outside the well, the two solutions should normally give the same result. However, the analytical method considers an aquifer of infinite areal extent which the numerical solution assumes a zero drawdown at the boundaries. In order to compare the two solutions, the method of images (Hantush, 1959; and Ferris et al., 1962) has been applied to the analytical solution to give a zero drawdown at the boundaries. Figure 6.9 shows the distribution of the images. The square at the center represents the area simulated with a producing well (sink represented by a negative sign (-)) at its center; the surrounding squares represent the images with a well (source if the sign is positive (+) and sink if the sign is negative (-)) at their center. The combined effect of a source and a sink of equal strength at points situated at equal distance from them is evidently zero. Figure 6.10 shows the corrected Hantush analytical solution and the numerical solution of the drawdown distribution along the x axis in the pumpage and in the lower zone. The two solutions compare very well outside the well-node as expected. Thus,

Table 6.26 Parameter Values for the Verification of the Drawdown Distribution

Parameter	Value
Q	1417.252 m^3/day
BU	76.2 m (250 feet)
BP	76.2 m
BL	76.2 m
BS	76.2 m
$K_h = K_z$	0.993 m/day
S_o	3.281 (10^{-6}) m^{-1}
n	0.3
DX	76.2 m

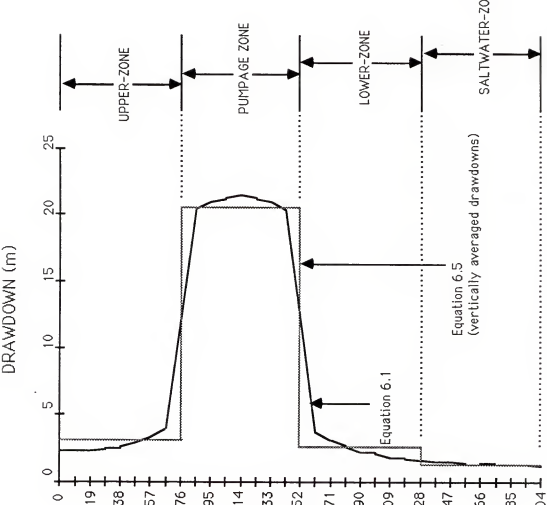
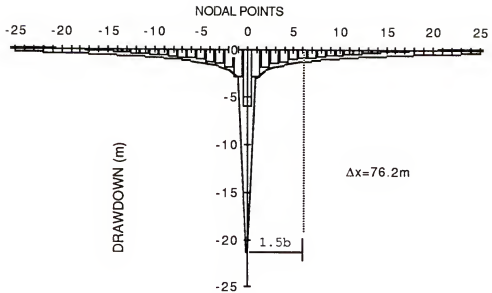
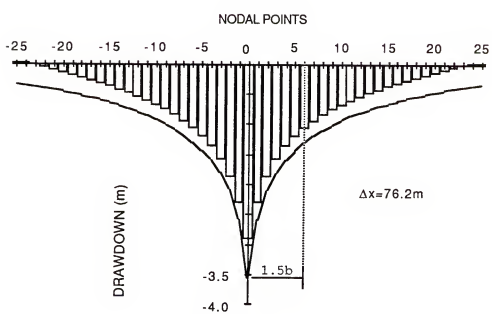


Figure 6.7 Vertical Distribution of the Drawdowns at the Well Node (Hantush's Analytical Solutions)



a. Pumpage-Zone



b. Lower-Zone

Figure 6.8 Comparison of the Numerical and the Analytical Drawdown Distribution (Without Correction)

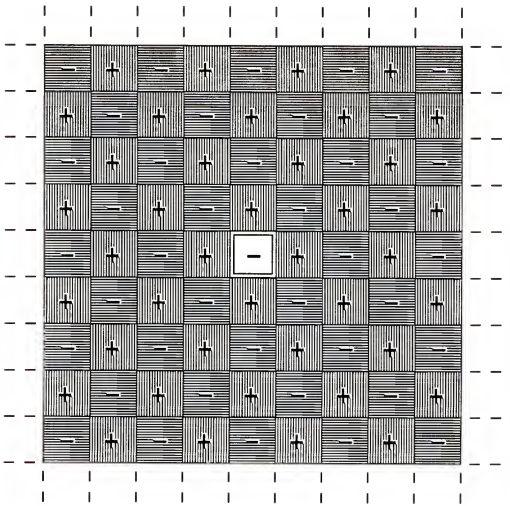
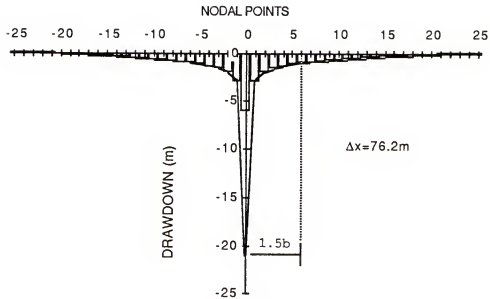
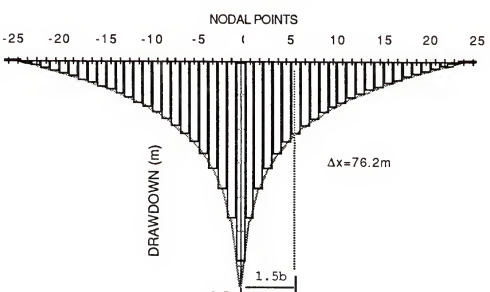


Figure 6.9 The Image Wells Distribution for the Correction of the Hantush's Analytical Drawdown Distribution



a. Pumpage-Zone



b. Lower-Zone

Figure 6.10 Comparison of the Numerical and the Analytical Drawdown Distribution After Correction by the Method of Images

the numerical solution of the flow equation is verified. The effect of smaller grid size (Δx) has been analyzed; several Δx's have been used and the results show that the numerical solution compares very well with the analytical solution outside the well node. Figure 6.11 shows the shape of the drawdown distribution using Δx = 15.24 m (50 feet).

6.4 Verification of the Saltwater Rise, Z_b

The phenomenon of upconing produced by pumping a liquid underlain by a denser liquid has long been recognized in the study of multiphase flow. Muskat (1946) analyzed the upconing of water under an oil producing well. Bear and Dagan (1968) have studied the case of sea water upconing below a freshwater producing well, using the theory of a sharp interface between the two fluids. Their solution, as reported by Schmorak and Mercado (1969), has the form

$$Z_{BD}(r,t) = \frac{Q}{2\pi(\Delta\gamma/\gamma_f)K_x BL}\left\{\frac{1}{(1+R^{12})^{1/2}} - \frac{1}{[(1+\gamma')^2+R^{12}]^{1/2}}\right\} \qquad (6.6)$$

where

Z_{BD} = rise of the interface above its initial position (L);

Q = pumping rate at the well (L^3T^{-1});

$\frac{\Delta\gamma}{\gamma_f}$ = dimensionless density difference between the two fluids (same as the density ratio factor ξ);

BL = distance between the well's bottom and the interface at t=0 (same as the thickness of the lower layer);

r = distance from the well;

$$R' = \frac{r}{BL}\left(\frac{K_z}{K_x}\right)^{1/2} \qquad (6.7)$$

$$\gamma' = \frac{(\Delta\gamma/\gamma)\,K_z}{2n \cdot BL}\,t \qquad (6.8)$$

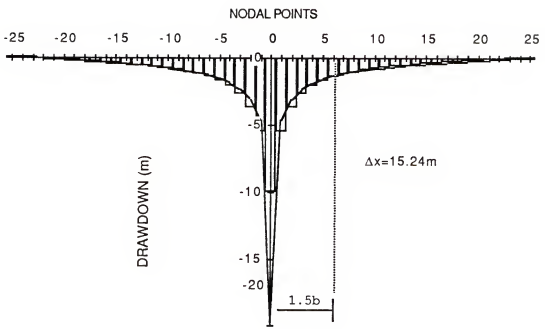


Figure 6.11 Comparison of the Numerical and the Corrected Analytical Drawdown Solution Using Small Δx

with R' = dimensionless distance from the well;

γ' = dimensionless time;

n = porosity of the aquifer;

K_x = horizontal hydraulic conductivity (LT^{-1});

K_z = vertical hydraulic conductivity (LT^{-1});

t = time elapsed since start of pumping (T).

Figure 6.12 shows the conceptual representation of the problem. For r=0, just below the pumping well, Equation 6.6 can be transformed into the form:

$$Z_{BD}(t)_{r=0} = \frac{Q}{2\pi(\Delta\gamma/\gamma_f)\, K_x BL}\left(1 - \frac{1}{1+\gamma'}\right) \qquad (6.9)$$

The assumptions underlying the development of Equation 6.6 were that

(a) the porous medium is homogeneous and nondeformable;

(b) the two fluids are incompressible and immiscible (separated by a sharp interface), and they obey Darcy's law;

(c) the aquifer is relatively thick;

(d) the screened portion of the well (BP) is small compared to BL (the distance between the bottom of the well and the initial position of the interface);

(e) the thickness BL is very small compared to both BU (the thickness of the freshwater above the screened portion of the well) and BS (the thickness of the saltwater underlying the freshwater).

Model experiments (Schmorak and Mercado, 1969) show that for values of (Z_{BD}/BL) greater than 1/3 to 2/3, the rate of rise of Z_{BD} is accelerated and at a certain critical rise, it reaches the bottom of the pumping well with a sudden jump. In order to compare the solution from

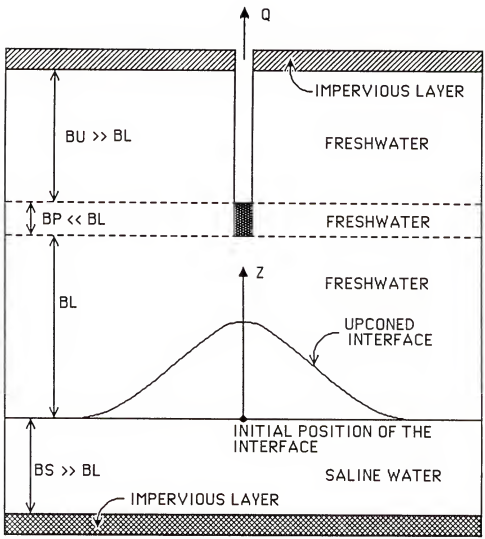


Figure 6.12 Conceptual Aquifer's Representation for Bear and Dagan's Saltwater Rise Solution

Equation 6.6 with the numerical solution, it has been assumed that the saltwater rise Z_{BD} equals (BL/3) after a 10-year period and BL has been estimated from Equation 6.6. The term "small" has been quantified in terms or ratios ($\frac{BP}{BL}$ and $\frac{BL}{BU}$). Two values (1/10 and 1/20) have been used for the ratio so that two sets of values have been used for BP, BU, and BS:

Case A: BU = BS = 1327.58 m; BP = 3.319 m

Case B: BU = BS = 663.793 m; BP = 6.638 m

The values of the other parameters of the problem are as follows:

Q = 1,417.252 m^3/day

K_x = 0.993 m/day

K_z = 0.0842 m/day

n = 0.30

BL = 66.379 m

When the dispersion terms vanish, the term ZDT in the developed model is equivalent to the saltwater rise, Z_b. For the purpose of the comparison of the numerical model with Bear and Dagan's analytical solution, dispersivities as small as 3.048×10^{-6} m (10^{-6} feet) and 1.524×10^{-5} m (5×10^{-6} feet) have been used for both a_L and a_T; both simulations yield the same results. Figures 6.13 and 6.14 show the results of both the numerical (with Δx = 152.4 m) and the analytical solutions. It appears that the numerical solution compares adequately with the analytical solution at the well; outside the well node, the numerical model underpredicts the rise of the saltwater front. A similar difference has been observed between Bear and Dagan's analytical

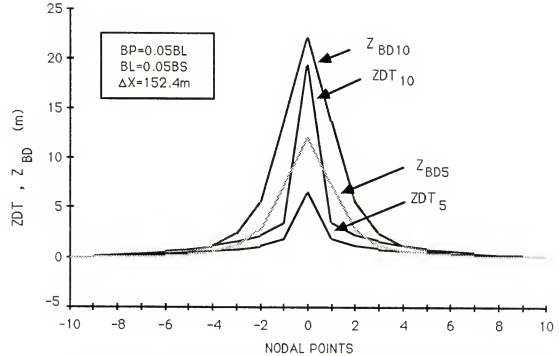


Figure 6.13 Comparison of the Numerical and the Bear and Dagan's Analytical Saltwater Rise Solutions With (BP/BL) = (BL/BS) = 1/20 and Δx = 152.4 m

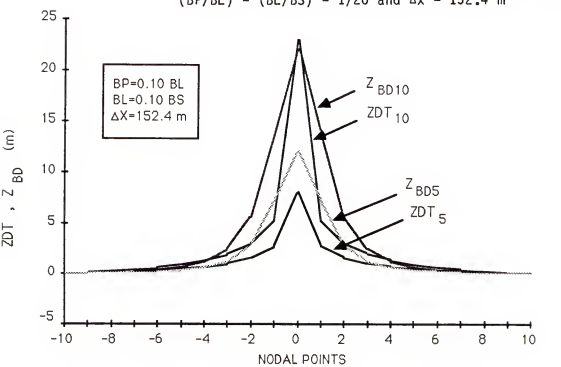


Figure 6.14 Comparison of the Numerical and the Bear and Dagan's Analytical Saltwater Rise Solutions With (BP/BL) = (BL/BS) = 1/10 and Δx 152.4 m

solution and a numerical sharp interface solution presented by Hoque (1983). Generally speaking, it can be concluded that the comparison between the analytical and the numerical solutions (of the saltwater rise, Z_b) presented on Figures 6.13 and 6.14 are satisfactory.

It can be speculated that the difference in shape between the two solutions is due to the conceptual formulation of the two models. While Bear and Dagan's method considers the well as a point-sink, the numerical method represents it by a finite-difference block. On the other hand, the assumption of a very thick saltwater layer infers non-horizontal flow in that zone and consequently no drawdown in the saltwater zone; under those circumstances, whatever is the drawdown in the lower zone, there will be a vertical flow between the fresh and saltwater zones, so that Z_b can still be important away from the well node. However, at a certain distance from the well, the numerical method gives the same drawdown in both the lower zone and the saltwater zone. Therefore, the vertical flow becomes zero at a certain distance from the well while the horizontal velocities might still be nonzero. The zero vertical velocity away from the well implies a zero rise of the saltwater front at that point. On the other hand, the horizontal velocities in the saltwater layer contribute to the importance of the vertical velocity just below the well, giving the shape of ZDT shown in Figures 6.13 through 6.16.

The question generally raised by the critics of the finite-difference method is the accuracy (with respect to the grid size Δx) of the method at a singularity such as a well. A horizontal finite-difference block size of Δx = 76.2 m has been used and yields the results shown in Figures 6.15 and 6.16. It seems that the rise of the saltwater obtained

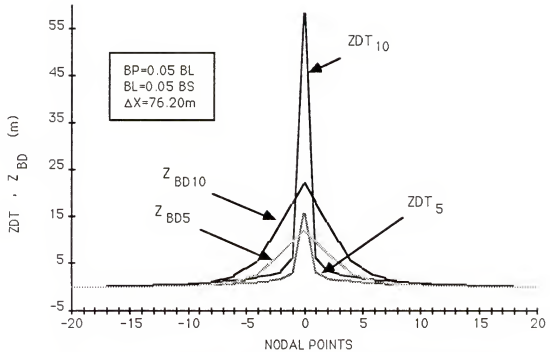


Figure 6.15 Comparison of the Numerical and the Bear and Dagan's Analytical Saltwater Rise Solutions With (BP/BL) = (BL/BS) = 1/20 and Δx = 76.2 m

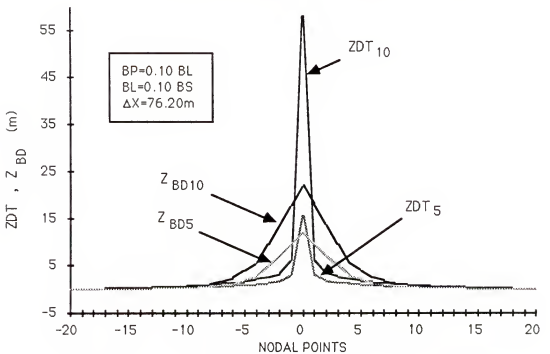


Figure 6.16 Comparison of the Numerical and the Bear and Dagan's Analytical Saltwater Rise Solutions With (BP/BL) = (BL/BS) = 1/10 and Δx = 76.2 m

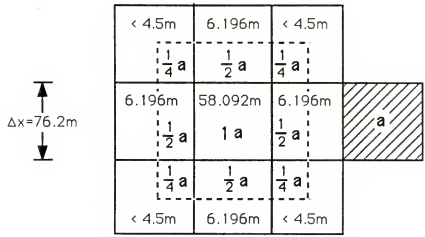
with small grid sizes is out of proportion, compared to the results of the analytical solution. However, from the comparison shown on Figure 6.17, it is evident that the average rise obtained from the simulation using $\Delta x = 76.2$ m is approximately the same as the rise obtained at the well using $\Delta x = 152.4$ m. On the other hand, the results shown in Figures 6.12 and 6.13 seem to indicate a better approximation at the well. The use of $\Delta x = 152.4$ m should therefore be preferred to the use of $\Delta x = 76.2$ m for the case studied here.

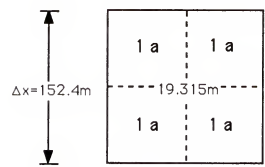
6.5 Application of the Model to the Simulation of a Wellfield

Brevard, Indian River, Osceola, and Volusia Counties (Figure 6.18) are in the east central region of Florida. Even though Osceola is not directly on the Atlantic Coast as are the others, its distance from the coast is relatively small and its aquifers can also be classified as coastal aquifers. Those four counties of the southern end of the St. John's River Water Management District rely on groundwater resources as their primary freshwater supply.

The region is growing very fast, and so is the water demand (Brown et al., 1962). The saline contamination in the eastern counties of Florida was detected early in the century (Sellards and Gunter, 1913). Since then, many investigations have been conducted (Collins and Howard, 1928; Black and Brown, 1951; and Munch et al., 1979). However, none of the existing studies has approached the well-contamination problem as it is done in the present work.

Matson and Sanford (1913) and Sellards and Gunter (1913) gave a general description of the water bearings in the concerned area. Their reports suggest fairly uniform layers with variable thickness and slope





$a = (76.2\ m)^2$ = unit horizontal area of a finite-difference block with $\Delta x = 76.2$ m

58.092 m = rise of the saltwater front in the block

$$\overline{ZDT} = \frac{(58.092)a + 3(6.196)a}{4a} = 19.70\ m$$

Figure 6.17 Comparison of the Saltwater Rise Around the Well Using Δx = 76.2 m and Δx = 152.4 m

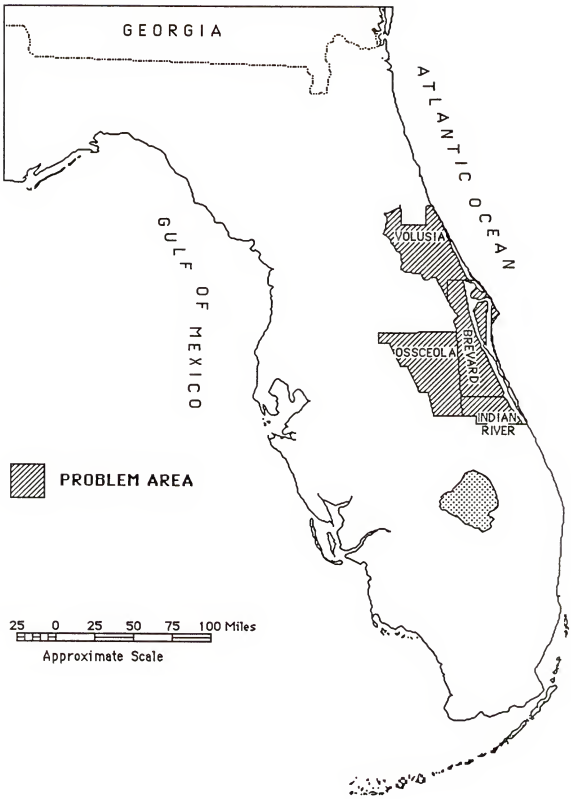


Figure 6.18 General Location of the Problem Area

for the water bearing formations in eastern Florida. However, Sellards and Gunter (1913) suggested referring to local details for a better appreciation of the geologic formations. The aquifers in the problem area, from the existing information, can be represented schematically by Figure 6.19 (type A aquifers) or Figure 6.20 (type B aquifers). In some cases, type B aquifers can simply be represented as shown in Figure 6.21. The structure of the aquifer systems in the concerned area can become very complex, consisting of the superposition of type A and B aquifers with wells pumping from different levels. Those complex aquifers will be called multiaquifer systems (Figure 6.22).

The model presented here can be modified to also simulate multiaquifer systems. The main change in the conception of such a model would be the consideration of a larger number of zones (vertical discretization of the aquifer system), instead of the simple four-zone model (upper-zone, pumpage-zone, lower-zone, and saltwater zone) considered by UPCON. However, since the modeling of a complex system is generally its approximation by a simplified system which is easier to analyze mathematically, UPCON can be used to simulate all of the aquifers presented in Figures 6.19 through 6.21. Nevertheless, while using UPCON, one should keep in mind the status of the actual aquifer system and all the necessary assumptions made in developing UPCON; this will help in the interpretation of the final results. For instance, in UPCON, the vertical velocity q_{z_o} at the boundary between the lower zone and the saltwater zone has been computed as

$$q_{z_o} = K_z \frac{(sL - sS)}{.5(BL + BS)} \tag{6.10}$$

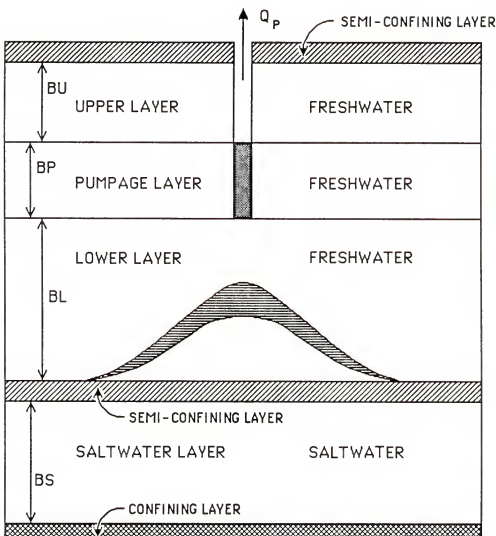


Figure 6.19 Conceptual Representation of a Coastal Aquifer With a Semi-Confining Bed Between the Freshwater and the Saltwater (Type-A Aquifer)

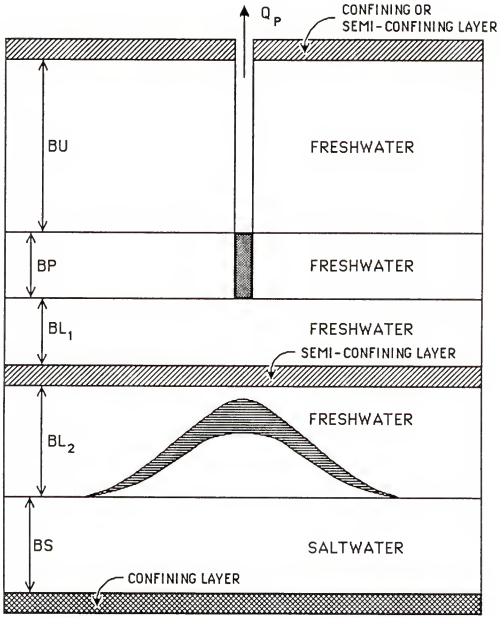


Figure 6.20 Conceptual Representation of a Coastal Aquifer With a Semi-Confining Bed Within the Freshwater (Type-B Aquifer)

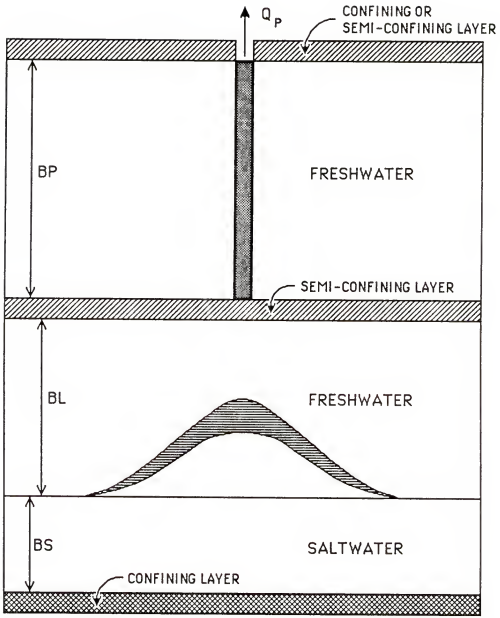


Figure 6.21 Simplified Representation of a Type-B Coastal Aquifer

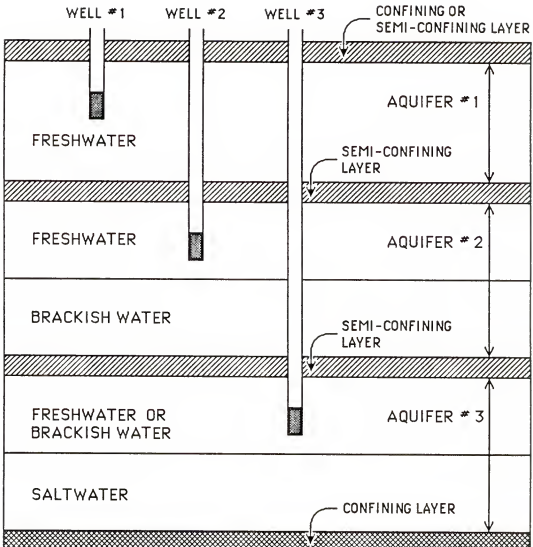


Figure 6.22 Multiaquifer System

while the same velocity in the simulation of type A aquifers should be evaluated by

$$q_{z_o} = K'_{z_s} \frac{(sL - sS)}{B'_s} \tag{6.11}$$

K'_{z_s} and B'_s are, respectively, the vertical hydraulic conductivity and the thickness of the semi-confining layer between the lower layer and the saltwater layer (see Figure 6.19). Defining σ, an analogous term to what Prickett and Lonnquist (1971) called a recharge factor,

$$\sigma_1 = \frac{K_z}{.5(BS + BL)} \tag{6.12}$$

$$\sigma_2 = \frac{K'_{z_s}}{B'_s} \tag{6.13}$$

it is evident that Equations 6.10 and 6.11 would be equivalent if $\sigma_1 = \sigma_2$. Bear (1979) defined σ_2 as the resistance of the semimpermeable layer. Since the vertical velocity q_{z_o} has an important effect on the vertical movement of the salt under the wells, a well-advised user can replace σ_1 by σ_2 in the model if the details of the type-A aquifer's characteristics are available. In a case where those details are not known (which is the most usual case), the user should keep in mind that Expression 6.13 is being approximated by Equation 6.12. The above discussion is an example of the type of problem the user of UPCON might face in the analysis of the result given by UPCON. Nevertheless, the effectiveness of the use of any model is a matter of experience, and any experienced groundwater hydrologist would be helpful in the interpretation of the results given by UPCON. The following is an example of the simulation of a multiple well system using UPCON.

The purpose of the analysis is not to predict the evolution of the well contamination in the considered area, but to demonstrate the capability of UPCON to simulate a non-homogeneous and anisotropic aquifer with multiple wells. The considered area is the Titusville wellfield in Brevard County, Florida. The available information on the considered wellfield is not sufficient to attempt in the present work the study of the evolution of contamination by the underlying saltwater. For instance, the history of the wellfield operation is not known; therefore, the history of the wells contamination cannot be considered for the calibration of the model.

The details of the geology of the Titusville area have been obtained mostly from well drilling information. The State of Florida is underlain by the Vicksburg limestones of Eocene age (Sellards and Gunter, 1913). The sediments overlying the limestones in the Titusville area are a lower marl ranging from 50 to 150 feet thick, and an upper sand ranging from 0 to 50 feet (Reynolds, Smith, and Hills; 1982). Locally, the marl has lenses of sand, shell, clay and sandy clay. The interrelationships of those sediments are complex, and a succession of the clay and or sandy clay lenses between the marl and the sand deposits form a layer acting like a semi-confining bed between the two deposits. The concerned aquifer can be classifed somewhere between type A and type B aquifers. However, it can be approximated by the conceptual aquifer (Figure 4.2) on which the development of UPCON is based.

Reynolds, Smith, and Hills (1982) reported that the known transmissivities in the Titusville area range from 3,000 to 8,300 gpd/ft and the storage coefficients range from 0.0001 to 0.0012. Those are values

in the area around the airport (wells #1 to #25). They also estimated the transmissivity of wells along the Interstate 95, to be about 24,000 gpd/ft. The values above can only serve as guidelines in the determination of the detailed characteristic values of the aquifer, the hydraulic conductivities, specific storage coefficients, and the thicknesses defined in UPCON (BU, BP, BL, and BS). It should be pointed out that the extent of the saltwater underlying the concerned area has not been mentioned in any of the existing reports. This is probably due to the cost of the investigation needed to determine the position of the saltwater front, as well as its extent. Tables 6.27 and 6.29 give the description of the "INPUT-DATA" to UPCON.

The lengths of the screened portion of the wells (BP) are obtained from the St. John's River Water Management District (Palatka, Florida); the pumping rates (Q), the observed drawdown (SACT), and the chloride content (CACT) are from the "Waterwell Master List" of the City of Titusville. Two illustrative simulations have been made. The first simulation considers the aquifer as 2 homogeneous "blocks" (Table 6.27) and the second considers 20 blocks (Table 6.29). The thickness of the freshwater in the aquifer is assumed to be about 200.01 feet; using the reported values of BP, the other thicknesses (BU and BL) have been approximated. The thickness of the saltwater layer has been assumed constant and equal to 130.01 feet. Finally, it is assumed that the whole wellfield has been in operation for 10 years, and the pumping rates have been constant over that period. This means that the chloride concentration at the wells are those observed 10 years after the wells have been in operation.

Table 6.27 Description of the Input Data: First Simulation

```
UPCONING DEVELOPMENT UNDER A WELL OR WELLFIELD
**********************************************

   THREE DIMENSIONAL ANALYSIS
   **************************

   INPUT DATA
   **********

     TITUSVILLE WELLFIELD SIMULATION
     PERIOD: 1-YEAR SIMULATION

     DEFAULT-VALUES
     **************

THE INPUT UNITS ARE: DAYS   MG/L     FT       FT/DAY  GPD
THE OUTPUT UNITS ARE: DAYS   MG/L     M         M/DAY  M**3/DAY

CONVERSION FACTORS: CF1= 0.13368  CF2= 0.30480

NW= 42   N= 37   M= 45  DI=   333.333 FT      DT1= 0.100E-01 DAYS     DTMAX=   20.00 DAYS     TMAX=   3650.00 DAYS

PRINTING LAGS IN  DAYS:
 DTP1=  3650.000  DPT1=  3650.000  DPT2=  7300.000  DPT3= 18250.000 PLC1=  3650.000  PLC2= 10950.000  PLC3= 36500.000
   THE TIME INCREMENT ACCELERATION FACTOR IS: 1.189

THICKNESS OF THE LAYERS IN FT
BM0=     3.000  BU0=    10.000  BP0=    56.180  BL0=   160.010  B50=   130.010

HYDRAULIC CONDUCTIVITIES IN FT/DAY
XKM=  0.134E-03  XKH0=  0.361E+02  XKV0=  0.430E-01
SPECIFIC STORAGE COEFFICIENT (STO) IN ( FT      **-1)  0.100E-05

PM=  0.300  AI=    21.840 FT        A2=     2.184 FT       CIN=   20.MG/L       CON0= 19000.MG/L
   B50= 0.000E+00 FT     / FT       S0=     0.00 FT        0L0=      0.00 FT       Z80=       0.00 FT
      RF0= 0.000E+00 FT/DAY

NODAL POINTS  WELL      SPECIFIC VALUES AT WELL NODES
  I       J     #        SACT        CACT          Q
                         FT          MG/L          GPD

  24     33   01.       29.50 '        28.      547200.
  24     29   03.       14.00          24.      187200.
  24     28   04.       16.50          20.      237600.
  24     27   05.       28.00          50.      115200.
  24     23   06.       23.50          34.      201600.
  25     31   08.       27.00         128.      172800.
  25     29   09.       32.00          42.      180000.
  29     29   11.       31.50         162.      100800.
  30     29   12.       24.50          60.      187200.
  21     31   13.        6.00         284.      230400.
  20     29   14.       39.00         595.      192960.
  24     35   15.       36.50         160.      280800.
  25     37   16.       18.50         226.      381600.
  26     35   17.       17.00         271.      309600.
  28     35   18.       43.00          38.      352800.
  30     35   19.       44.50         999.      374400.
  30     26   20.       10.50         364.      417600.
  30     24   21.       12.00          45.      504000.
  30     23   22.       26.50         216.      172800.
  29     22   23.       44.00         106.      273600.
  27     22   24.       42.00         160.      194400.
```

Table 6.27--Continued

NODAL POINTS I	J	WELL #	SPECIFIC VALUES AT WELL NODES SACT FT	CACT MG/L	Q GPD
20	33	26.	28.50	48.	259200.
17	33	27.	13.00	250.	288000.
18	30	28.	16.00	125.	194400.
16	29	29.	4.50	87.	43200.
15	29	30.	15.50	36.	158400.
17	26	31.	21.00	92.	453600.
15	26	32.	17.50	32.	244800.
14	26	33.	13.50	28.	158400.
13	24	34.	31.00	22.	360000.
13	23	35.	5.00	26.	266400.
12	21	36.	4.50	23.	331200.
12	20	37.	5.50	27.	288000.
11	18	39.	11.50	20.	288000.
10	17	40.	16.00	28.	122400.
9	14	42.	13.50	23.	324000.
10	13	43.	10.00	28.	345600.
9	12	45.	7.00	29.	360000.
8	11	46.	9.50	23.	230400.
8	9	47.	4.50	21.	43200.
7	8	48.	15.00	32.	252000.
7	7	49.	15.50	29.	216000.

NB= 2 ICAL= 6

SPECIFICATIONS FOR THE NON-HOMOGENEITY OF THE AQUIFER

BLOC#	I1	I2	J1	J2	BMO FT	BUO FT	BPO FT	BLO FT	BSO FT	XKMO FT/DAY	XKHO FT/DAY	XKVO FT/DAY	STO FT	(**-1)
1	19	37	1	45	3.000	10.000	86.955	113.045	130.010	0.134E-03	0.501E+02	0.836E-01	0.100E-05	
2	1	18	1	45	3.000	10.000	31.850	158.150	130.010	0.134E-03	0.217E+03	0.919E-01	0.100E-05	

Table 6.28 Results of the First Simulation

ESTIMATED VALUES AT THE WELLS (TIME=10 YEARS); (2-BLOCKS SIMULATION)

I	J	WELL #	RATIO 1	ACT.DRAW. (FEET)	EST. DRAW. (FEET)	OEL (FEET)	Z (FEET)	RATIO 2	ACT.CONC (PPM)	EST.CON. (PPM)
24	33	01.	0.88460	29.500	26.096	177.12	3.04	30.17	28.	845.
24	29	03.	1.69214	14.000	23.690	186.46	8.50	65.67	24.	1576.
24	28	04.	1.41377	16.500	23.327	180.20	7.60	58.55	20.	1171.
24	27	05.	0.74959	28.000	20.989	158.05	6.57	12.46	50.	623.
24	23	06.	0.72164	23.500	16.959	122.17	1.20	0.97	34.	33.
25	31	08.	0.84466	27.000	22.806	189.64	9.99	15.28	128.	1956.
25	29	09.	0.72327	32.000	23.145	227.14	6.61	58.69	42.	2465.
29	29	11.	0.57328	31.500	18.058	116.57	0.00	0.13	162.	21.
30	29	12.	0.70111	24.500	17.177	90.62	0.00	0.33	60.	20.
21	31	13	3.37303	6.000	20.238	108.25	0.00	0.08	284.	23.
20	29	14.	0.47639	39.000	18.579	97.97	0.00	0.03	595.	20.
24	35	15.	0.59943	36.500	21.879	126.53	0.00	0.30	160.	48.
25	37	16.	1.02408	18.500	18.945	90.30	0.00	0.09	226.	20.
26	35	17.	1.31284	17.000	22.318	143.44	0.48	0.79	271.	214.
28	35	18.	0.47668	43.000	20.497	115.26	0.00	0.66	38.	25.
30	35	19.	0.38415	44.500	17.095	75.71	0.00	0.02	999.	20.
30	26	20.	1.97629	10.500	20.751	102.15	0.00	0.08	364.	27.
30	24	21.	1.81807	12.000	21.817	97.81	0.00	0.52	45.	23.
30	23	22.	0.70340	26.500	18.640	84.03	0.00	0.09	216.	20.
29	22	23.	0.40539	44.000	17.937	92.04	0.00	0.19	106.	20.
27	22	24.	0.40436	42.000	16.983	112.63	0.11	0.13	160.	20.
20	33	26.	0.60477	28.500	17.236	70.55	0.00	0.42	48.	20.
17	33	27.	0.95222	13.000	12.379	41.07	0.00	0.08	250.	20.
18	30	28.	0.95051	16.000	15.208	62.54	0.00	0.16	125.	20.
16	29	29.	3.07340	4.500	13.830	55.78	0.00	0.23	87.	20.
15	29	30.	0.85541	15.500	13.259	50.15	0.00	0.56	36.	20.
17	26	31.	0.82429	21.000	17.310	79.85	0.00	0.22	92.	20.
15	26	32.	0.90706	17.500	15.874	63.00	0.00	0.63	32.	20.
14	26	33.	1.08841	13.500	14.694	54.25	0.00	0.71	28.	20.
13	24	34.	0.49141	31.000	15.234	51.78	0.00	0.91	22.	20.
13	23	35.	2.99656	5.000	14.983	52.62	0.00	0.77	26.	20.
12	21	36.	3.16019	4.500	14.221	45.99	0.00	0.87	23.	20.
12	20	37.	2.50492	5.500	13.777	45.41	0.00	0.74	27.	20.
11	18	39.	1.03662	11.500	11.921	37.95	0.00	1.00	20.	20.
10	17	40.	0.64590	16.000	10.334	30.81	0.00	0.71	28.	20.
9	14	42.	0.82164	13.500	11.092	24.98	0.00	0.87	23.	20.
10	13	43.	1.13388	10.000	11.339	29.35	0.00	0.71	28.	20.
9	12	45.	1.56639	7.000	10.965	22.66	0.00	0.69	29.	20.
8	11	46.	0.93396	9.500	8.873	16.89	0.00	0.87	23.	20.
8	9	47.	1.48806	4.500	6.696	14.01	0.00	0.95	21.	20.
7	8	48.	0.44784	15.000	6.718	10.08	0.00	0.63	32.	20.
7	7	49.	0.38038	15.500	5.896	8.08	0.00	0.69	29.	20.

Table 6.28 shows the result of the first simulation, using data from Table 6.27. RAT101 and RAT102 denote, respectively, the ratio of the calculated drawdown to the observed drawdown and the ratio of the calculated chloride concentration to that observed. Based on those ratios, the guessed values of the characteristics of the aquifer (K_H, K_Z, BU, BP, BS, etc.) can be adjusted in order to bring those ratios close to one. It should be noticed that the history of the wellfield contamination should be used in conjunction with RAT102 for the adjustments of those values. For instance, if well #1 has been in operation for 15 years, while well #19 has been in operation for 12 years, RAT102 for well #1 should equal 1 after 15 years of simulation, and RAT102 for well #19 should equal 1 after 12 years of simulation.

In Table 6.28, it can be seen that RAT101-values are more reasonable than those of RAT102. This is primarily due to the fact that the first approximation of the unknown input values is mainly based on the factors controlling the drawdowns, such as the thicknesses and the (horizontal) hydraulic conductivities. Considering the distributions of the wells on Figure 6.23, average values of RAT101 and RAT102 are used to correct the characteristics of the aquifer. Each average value defined another "block" within the existing blocks. This "trial and error process" leads to the second simulation with 20 blocks. Table 6.30 shows the results of that simulation. As can be seen, there is a great improvement in the values of RAT102. An important fact to notice is that the high values of RAT101 are observed at wells where the observed drawdowns are small compared to the others (e.g. wells #13, 29, 35, 36, 37, 45, 46, and 47). A possible explanation of that behavior is that the screened portion of some wells is intersected by clay lenses

Table 6.29 Description of the Input Data: Second Simulation

```
UPCOMING DEVELOPMENT UNDER A WELL OR WELLFIELD
**********************************************

   THREE DIMENSIONAL ANALYSIS
   **************************

   INPUT DATA
   **********

     TITUSVILLE WELLFIELD SIMULATION
     PERIOD: 1-YEAR SIMULATION

     DEFAULT-VALUES
     **************

THE INPUT UNITS ARE: DAYS   MG/L      FT       FT/DAY  GPD
THE OUTPUT UNITS ARE: DAYS   MG/L      M         M/DAY  M**3/DAY

CONVERSION FACTORS: CF1= 0.13368  CF2= 0.30480

NW= 42    N= 37    M= 45  DX=   333.333 FT      DTI= 0.100E-01 DAYS     DTMAX=   20.00 DAYS     TMAX=   3650.00 DAYS

PRINTING LAGS IN  DAYS:
 DTPR=  3650.000  DPT1=  3650.000  DPT2=  7300.000  DPT3= 18250.000 PLC1=  3650.000  PLC2= 10950.000  PLC3= 36500.000
  THE TIME INCREMENT ACCELERATION FACTOR IS: 1.189

THICKNESS OF THE LAYERS IN FT
BM0=     3.000  BU0=    10.000  BP0=    56.180  BL0=   160.010  B50=   130.010

HYDRAULIC CONDUCTIVITIES IN FT/DAY
 XKM=  0.134E-03  XKH0=  0.361E+02  XKV0=  0.430E-01
SPECIFIC STORAGE COEFFICIENT (STO) IN ( FT      **-1)  0.100E-05

PM=  0.300  A1=    21.840 FT       A2=     2.184 FT       CIM=   20.MG/L      COM0= 19000.MG/L
   050= 0.000E+00 FT      / FT      50=      0.00 FT       OL0=      0.00 FT      Z80=      0.00 FT
      RF0= 0.000E+00 FT/DAY

NODAL POINTS   WELL      SPECIFIC VALUES AT WELL NODES
   I      J     #          SACT        CACT          Q
                            FT          MG/L        GPD

  24     33    01.         29.50         28.     547200.
  24     29    03.         14.00         24.     187200.
  24     28    04.         16.50         20.     237600.
  24     27    05.         28.00         50.     115200.
  24     23    06.         23.50         34.     201600.
  25     31    08.         27.00        128.     172800.
  25     29    09.         32.00         42.     180000.
  29     29    11.         31.50        162.     100800.
  30     29    12.         24.50         60.     187200.
  21     31    13          6.00         284.     230400.
  20     29    14.         39.00        595.     192960.
  24     35    15.         36.50        160.     280800.
  25     37    16.         18.50        226.     381600.
  26     35    17.         17.00        271.     309600.
  28     35    18.         43.00         38.     352800.
  30     35    19.         44.50        999.     374400.
  30     26    20.         10.50        364.     417600.
  30     24    21.         12.00         45.     504000.
  30     23    22.         26.50        216.     172800.
  29     22    23.         44.00        106.     273600.
  27     22    24.         42.00        160.     194400.
```

Table 6.29--Continued

NODAL POINTS I	J	WELL #	SPECIFIC VALUES AT WELL NODES SACT FT	CACT MG/L	Q GPD
20	33	26.	28.50	48.	259200.
17	33	27.	13.00	250.	288000.
18	30	28.	16.00	125.	194400.
16	29	29.	4.50	87.	43200.
15	29	30.	15.50	36.	158400.
17	26	31.	21.00	92.	453600.
15	26	32.	17.50	32.	244800.
14	26	33.	13.50	28.	158400.
13	24	34.	31.00	22.	360000.
13	23	35.	5.00	26.	266400.
12	21	36.	4.50	23.	331200.
12	20	37.	5.50	27.	288000.
11	18	39.	11.50	20.	288000.
10	17	40.	16.00	28.	122400.
9	14	42.	13.50	23.	324000.
10	13	43.	10.00	28.	345600.
9	12	45.	7.00	29.	360000.
8	11	46.	9.50	23.	230400.
8	9	47.	4.50	21.	43200.
7	8	48.	15.00	32.	252000.
7	7	49.	15.50	29.	216000.

NB= 20 ICAL= 6

SPECIFICATIONS FOR THE NON-HOMOGENEITY OF THE AQUIFER

BLOC# I1	I2	J1	J2	BMO FT	BUO FT	BPO FT	BLO FT	BSO FT	XXMO FT/DAY	XXNO FT/DAY	XXVO FT/DAY	STO FT (**-1)
1	19	37	1	45	3.000	10.000	86.955	113.045	130.010	0.134E-03	0.501E+02	0.836E-01	0.100E-05
2	1	18	1	45	3.000	10.000	31.850	158.150	130.010	0.134E-03	0.217E+03	0.919E-01	0.100E-05
3	23	25	32	33	3.000	10.000	86.955	113.045	130.010	0.134E-03	0.501E+02	0.219E-01	0.100E-05
4	23	24	28	29	3.000	10.000	86.955	113.045	130.010	0.134E-03	0.825E+02	0.271E-01	0.100E-05
5	23	25	26	27	3.000	10.000	86.955	113.045	130.010	0.134E-03	0.501E+02	0.338E-01	0.100E-05
6	24	26	30	31	3.000	10.000	86.955	113.045	130.010	0.134E-03	0.501E+02	0.338E-01	0.100E-05
7	25	26	29	29	3.000	10.000	86.955	113.045	130.010	0.134E-03	0.501E+02	0.200E-01	0.100E-05
8	28	30	28	29	3.000	10.000	86.955	113.045	130.010	0.134E-03	0.501E+02	0.919E-01	0.100E-05
9	20	22	30	32	3.000	10.000	90.000	110.000	130.010	0.134E-03	0.179E+03	0.121E+00	0.100E-05
10	19	21	28	29	3.000	10.000	66.955	113.045	130.010	0.134E-03	0.125E+02	0.116E+00	0.100E-05
11	23	24	34	36	3.000	10.000	86.955	113.045	130.010	0.134E-03	0.301E+02	0.743E-01	0.100E-05
12	27	28	34	36	3.000	10.000	106.955	163.045	130.010	0.134E-03	0.921E+01	0.300E-01	0.100E-05
13	29	32	33	37	3.000	10.000	123.000	77.000	130.010	0.134E-03	0.495E+01	0.846E-01	0.100E-05
14	28	33	24	26	3.000	10.000	86.955	113.045	130.010	0.134E-03	0.102E+03	0.116E+00	0.100E-05
15	26	32	20	23	3.000	10.000	86.955	113.045	130.010	0.134E-03	0.861E+01	0.558E-01	0.100E-05
16	16	17	28	30	3.000	10.000	31.850	158.150	130.010	0.134E-03	0.691E+03	0.929E-01	0.100E-05
17	12	14	24	25	3.000	10.000	31.850	158.150	130.010	0.134E-03	0.110E+03	0.929E-01	0.100E-05
18	10	14	19	23	3.000	10.000	31.850	158.150	130.010	0.134E-03	0.644E+03	0.929E-01	0.100E-05
19	7	11	9	13	3.000	10.000	31.850	158.150	130.010	0.134E-03	0.284E+03	0.929E-01	0.100E-05
20	5	9	5	8	3.000	10.000	31.850	158.150	130.010	0.134E-03	0.917E+02	0.929E-01	0.100E-05

Table 6.30 Results of the Second Simulation

ESTIMATED VALUES AT THE WELLS (TIME=10 YEARS); (20-BLOCKS SIMULATION)

I	J	WELL #	RATIO 1	ACT.DRAW. (FEET)	EST. DRAW. (FEET)	DEL (FEET)	Z (FEET)	RATIO 2	ACT.CONC (PPM)	EST.CON. (PPM)
24	33	01.	0.96692	29.500	28.524	68.42	0.00	8.47	28.	237.
24	29	03.	1.72901	14.000	24.206	75.74	0.00	37.87	24.	909.
24	28	04.	1.45053	16.500	23.934	63.01	0.00	17.25	20.	345.
24	27	05.	0.79470	28.000	22.251	74.80	0.00	0.94	50.	47.
24	23	06.	0.74558	23.500	17.521	123.14	0.72	0.98	34.	33.
25	31	08.	0.91095	27.000	24.596	86.58	0.00	1.86	128.	239.
25	29	09.	0.76537	32.000	24.492	43.17	0.00	7.93	42.	333.
29	29	11.	0.61502	31.500	19.373	137.78	1.93	0.93	162.	151.
30	29	12.	0.74733	24.500	18.310	104.51	0.00	0.33	60.	20.
21	31	13	3.23823	6.000	19.429	116.52	0.00	0.10	284.	27.
20	29	14.	0.53006	39.000	20.672	174.49	4.59	1.17	595.	696.
24	35	15.	0.68642	36.500	25.054	129.86	0.14	0.45	160.	72.
25	37	16.	1.07949	18.500	19.971	91.65	0.00	0.09	226.	20.
26	35	17.	1.53070	17.000	26.022	147.34	0.18	1.46	271.	396.
28	35	18.	0.86153	43.000	37.046	50.89	0.00	22.11	38.	840.
30	35	19.	0.93123	44.500	41.440	378.33	28.80	3.79	999.	3783.
30	26	20.	1.90451	10.500	19.997	125.74	0.00	0.38	364.	139.
30	24	21.	1.83291	12.000	21.995	107.30	0.00	5.54	45.	249.
30	23	22.	0.91853	26.500	24.341	102.62	0.06	0.75	216.	161.
29	22	23.	0.73142	44.000	32.182	114.12	0.00	1.80	106.	191.
27	22	24.	0.65055	42.000	27.323	111.43	0.16	0.61	160.	98.
20	33	26.	0.63015	28.500	17.959	69.71	0.00	0.42	48.	20.
17	33	27.	0.99274	13.000	12.906	41.87	0.00	0.08	250.	20.
18	30	28.	0.93939	16.000	15.030	65.20	0.00	0.16	125.	20.
16	29	29.	3.05487	4.500	13.747	56.18	0.00	0.23	87.	20.
15	29	30.	0.87220	15.500	13.519	51.05	0.00	0.56	36.	20.
17	26	31.	0.79648	21.000	16.726	81.24	0.00	0.22	92.	20.
15	26	32.	0.88369	17.500	15.465	67.18	0.00	0.63	32.	20.
14	26	33.	1.06240	13.500	14.342	58.82	0.00	0.71	28.	20.
13	24	34.	0.47124	31.000	14.608	53.71	0.00	0.91	22.	20.
13	23	35.	2.69096	5.000	13.455	45.08	0.00	0.77	26.	20.
12	21	36.	2.69927	4.500	12.147	42.35	0.00	0.87	23.	20.
12	20	37.	2.17709	5.500	11.974	42.13	0.00	0.74	27.	20.
11	18	39.	1.02114	11.500	11.743	43.82	0.00	1.00	20.	20.
10	17	40.	0.65486	16.000	10.478	32.59	0.00	0.71	28.	20.
9	14	42.	0.81630	13.500	11.020	26.50	0.00	0.87	23.	20.
10	13	43.	1.08937	10.000	10.894	29.80	0.00	0.71	28.	20.
9	12	45.	1.50930	7.000	10.565	24.47	0.00	0.69	29.	20.
8	11	46.	0.94301	9.500	8.959	18.73	0.00	0.87	23.	20.
8	9	47.	1.69524	4.500	7.629	18.09	0.00	0.95	21.	20.
7	8	48.	0.61646	15.000	9.247	15.60	0.00	0.63	32.	20.
7	7	49.	0.54487	15.500	8.446	10.05	0.00	0.69	29.	20.

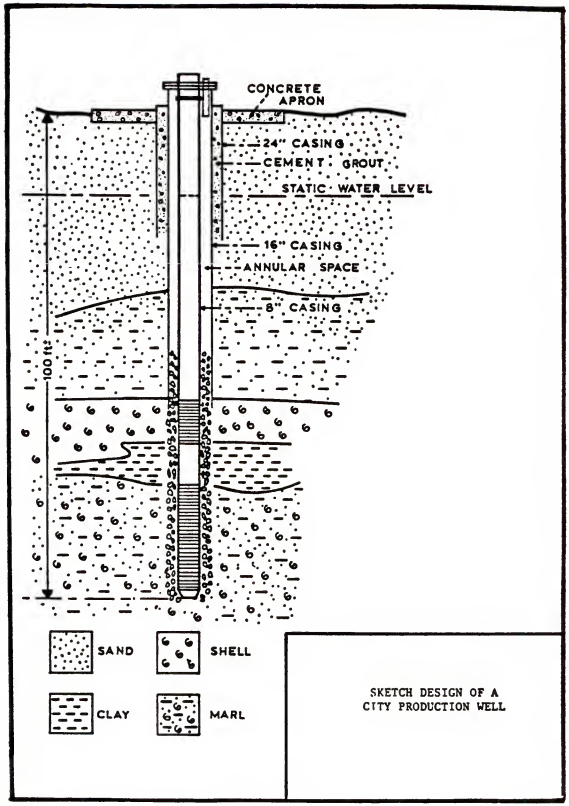


Figure 6.23 Production Well With Double Screened Portions

(Figure 6.23), and therefore, the observed drawdowns at those wells are not necessarily the actual ones. Also, a low chloride concentration in a well with a large drawdown (e.g., well #18) can be explained by the presence of a clay lens below the well (in the lower zone) and acting as a "protector-screen" to the well. The role of such a lens would be to diffuse the transition zone laterally, and to reduce the vertical movement of the salt toward that zone. The resulting effect of the lateral movement of the transition zone would be the transfer of salt from below the protected well to adjacent wells. Figures 6.24 through 6.29 show the mapping format used in UPCON to present the results of a simulation.

The analysis of the predicted concentration is rather difficult since the history of the contamination is not known. However, the results in Tables 6.29 through 6.33 show that UPCON is capable of simulating complex aquifer systems such as that in Titusville area.

MAP OF THE WELLFIELD

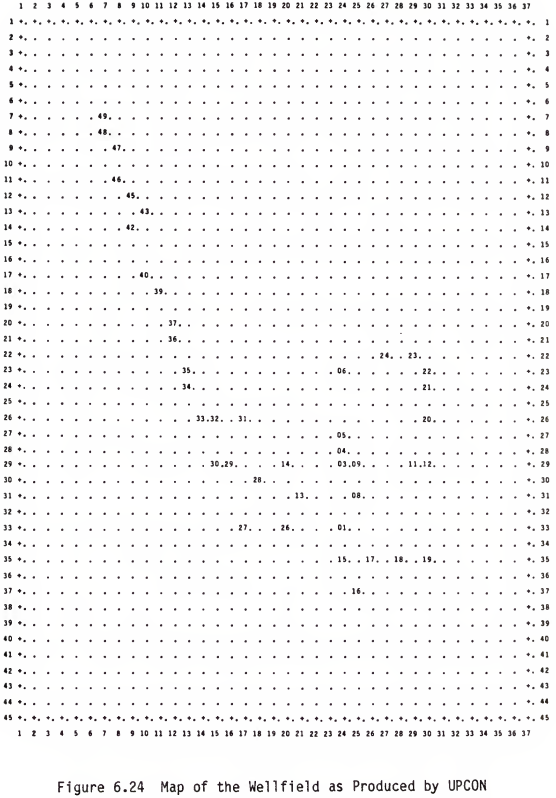


Figure 6.24 Map of the Wellfield as Produced by UPCON

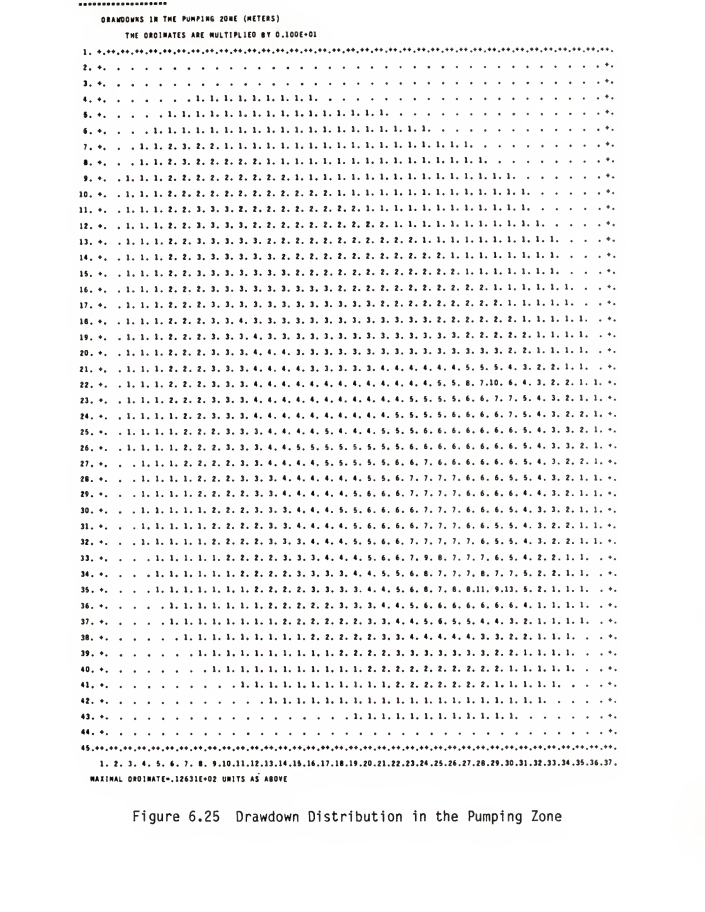

T= 0.3650DE+04 DAYS
DRAWDOWNS IN THE PUMPING ZONE (METERS)
THE ORDINATES ARE MULTIPLIED BY 0.100E+01
1. 2. 3. 4. 5. 6. 7. 8. 9.10.11.12.13.14.15.16.17.18.19.20.21.22.23.24.25.26.27.28.29.30.31.32.33.34.35.36.37.
MAXIMAL ORDINATE=.12631E+02 UNITS AS ABOVE

Figure 6.25 Drawdown Distribution in the Pumping Zone

```
T= 0.36500E+04 DAYS
**********

     DRAWDOWNS IN THE LOWER ZONE (METERS)

          THE ORDINATES ARE MULTIPLIED BY 0.100E+02

 1. +.+.+.+
```

```
T= 0.3650DE+04 DAYS
********************

     DRAWDOWNS IN THE SALTWATER ZONE (METERS)

          THE ORDINATES ARE MULTIPLIED BY 0.10DE+03

 1. +.**.**.**
```

```
T= 0.365DDE+04 DAYS
==================

    MAP OF ZDT  (METERS)

        THE ORDINATES ARE MULTIPLIED BY 0.100E+01

 1. +.**.**.**
```

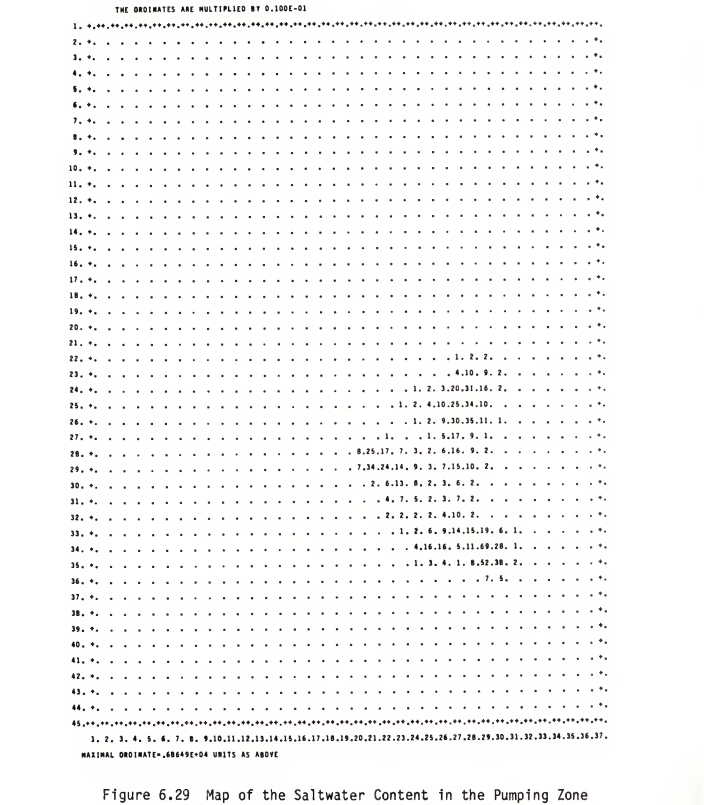

T= 0.3650DE+04 DAYS
CONCENTRATIONS IN THE PUMPING ZONE (MG/LIT)
THE ORDINATES ARE MULTIPLIED BY 0.100E-01
1. 2. 3. 4. 5. 6. 7. 8. 9.10.11.12.13.14.15.16.17.18.19.20.21.22.23.24.25.26.27.28.29.30.31.32.33.34.35.36.37.
MAXIMAL ORDINATE=.6864 9E+04 UNITS AS ABOVE

Figure 6.29 Map of the Saltwater Content in the Pumping Zone

CHAPTER 7
SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS FOR FUTURE WORK

7.1 Summary

Saltwater upconing under a producing well pumping from a coastal region aquifer is a classical result of underground water development in those areas. Previous studies of the intrusion of saltwater into freshwater assume a sharp interface between the two fluids, neglecting the effect of the hydrodynamic dispersion which creates a transition zone between the freshwater and the saltwater. The present work describes a numerical model that simulates the upconing phenomenon more accurately and more effectively.

A three-dimensional numerical model written in standard FORTRAN has been developed for simulating the upconing phenomenon under a producing well in a coastal aquifer. The model is capable of simulating aquifer systems with homogeneous/non-homogeneous, isotropic/anisotropic conditions, and leaky/non-leaky confined aquifer. The model can easily be adapted to also simulate non-confined aquifers.

A finite difference method has been used to approximate the partial differential equations describing the flow system and the transport phenomena in the aquifer system. The "Alternating Direction Iterative" (ADI) method is used to solve the three-dimensional partial difference equations.

The performance of the numerical model has been evaluated by comparing its solution with some existing analytical solutions and by

applying the model to simulate Titusville (Brevard County, Florida) wellfield where well contamination by underground saltwater is a threat to the groundwater development.

In the development of UPCON (the model described herein), emphasis has been put on the three-dimensional representation of the aquifer system and on the effective representation of the contamination process mainly controlled by the hydrodynamic dispersion.

7.2 Conclusions

The analysis of the performance of the model shows that UPCON is reasonably efficient in simulating the upconing phenomenon under a producing well (or well field) pumping from a coastal aquifer underlain by saltwater. In particular,

- the model shows that the "sharp interface theory" does not apply in the study of the upconing phenomenon under a pumping well; for the well is contaminated long before the saltwater front reaches the bottom of the well;
- the model accurately represents the drawdown distribution induced by a well partially penetrating a leaky/non-leaky confined aquifer;
- the model accurately represents the three-dimensional flow in a coastal aquifer subject to pumping and underlain by saltwater;
- the model reasonably represents the transition zone and the saltwater mound under the well;
- the model gives an acceptable representation of the chloride distribution in the pumping region;

- the model shows that the factors which mostly influence the chloride contamination process are:
  (a) the horizontal and vertical hydraulic conductivities;
  (b) the length of the screened portion of the well;
  (c) the distance between the bottom of the well and the initial position of the saltwater front; and
  (d) the thickness of the saltwater underlaying the freshwater.

7.3 Recommendation for Future Work

It is generally assumed that saltwater is a homogeneous fluid with a constant chloride content (about 35 g/l). The results from the present study (see Appendix B) suggest that the chloride distribution in underground saltwater might not be uniform. Furthermore, the actual transition zone might need to be redefined. On the other hand, the values of the dispersivities (a_L and a_T) are almost nonexistent. Nevertheless, the reliability of the simulation of the upconing phenomenon greatly depends on those values. Those limitations do not allow the study of the upconing in more complex aquifer systems such as multiaquifer systems (see Section 6.5).

The following analyses will enhance the performance of the model herein described.

(1) The study of the chloride distribution in underground saltwater underlying freshwater in coastal aquifer.

This study will improve the understanding of the chloride distribution in underground saltwater and help in the redefinition of the top of the saltwater zone. The chloride content in underground saltwater varies from 19 g/l to 21 g/l according to the

existing information on the topic. However, the standard chloride content in saltwater is 35 g/l and from the definition of the transition zone (zone of chloride content varying from that of saltwater at the bottom to that of freshwater at the top), most of underground saltwater considered in the literature is part of the transition zone and in some cases, the saltwater may not even exist.

(2) The study of the chloride distribution in the transition zone, the boundary between the freshwater and the saltwater with and without pumpage.

The "sharp interface theory" stems from the fact that the thickness of the transition zone is very small when the vertical flow component is negligible compared to the horizontal ones in the underground flow field. Many studies being based on the "sharp interface theory" (see Chapter 2) suggest that that approach is not completely unacceptable under the specified conditions. The present work assumed a sharp interface for the initial position of the saltwater front. However, the Floridian aquifers (mainly the Biscayne, south of Miami; Henry 1964a; Segol and Pinder, 1976) are well known for having a significant mixing zone (transition zone). The existing theories on the transition zone do not consider the effect of pumping on the chloride profile in the transition zone.

The suggested study will provide a better representation of the influence function describing the chloride distribution in the transition zone of the upconing due to pumpage.

(3) The study of the dispersivities in the Floridian aquifers will, certainly, enhance the reliability of the UPCON performance.

(4) The modification of the current version of UPCON is in order to analyse the degree of importance of the the error(s) made by representing a multiaquifer system by the conceptual aquifer modeled by UPCON.

APPENDIX A
DERIVATION OF THE FUNCTION OF THE DENSITY $\rho = \rho(c)$

Derivation of Function of the Density $\rho(c)$

The relationship between the freshwater density ρ_f and the chloride concentration c^* has been investigated by different authors. Pinder and Cooper (1970) reported an empirical relationship (developed by Baxter and Wallace, 1916) relating water density ρ and chloride concentration c as follows:

$$\rho = \rho_o + (1 - E)\, c^* \tag{A.1}$$

where

ρ_o = reference density of water

c^* = actual chloride concentration

ρ = density of water with chloride solution

E - is about 0.3 for concentration to as much as that of seawater (Pinder and Cooper, 1970)

Rubin and Pinder (1977) related the water density ρ and the chloride concentration c by

$$\rho = \rho_o(1 + \alpha c^*) \tag{A.2}$$

where α is a coefficient

Rewriting Equation A.1 as

$$\rho = \rho_o\left[1 + \frac{(1 - E)}{\rho_o}\, c^*\right] \tag{A.3}$$

it can be seen that both Equation A.1 and A.2 have the same form and that they are equivalent when

$$\alpha = \frac{1 - E}{\rho_0} \tag{A.4}$$

However, it should be noticed that

1. No freshwater has the reference density ρ_0. Any ground freshwater has a certain content of chloride.

2. Seawater generally contains different kinds of dissolved minerals and the density of seawater is different from that of an ideal water containing NaCl only.

The purpose of the analysis which follows is therefore to derive an expression which can be used to approximate the relationship between ρ, the density of a water with a certain amount of chloride concentration c^* , and ρ_f, the density of a freshwater of known concentration c_f^*.

Application of Equation A.2 to the freshwater density gives

$$\rho_f = \rho_0(1 + \alpha c_f^*) \tag{A.5}$$

Subtraction of Equation A.5 from A.2 yields

$$\rho - \rho_f = \rho_0 \alpha(c^* - c_f^*) \tag{A.6}$$

Dividing Equation A.6 by A.5 and assuming that $1 + \alpha c_f^*$ is approximately equal to 1.0 (the maximum value of $1 + \alpha c_f^*$ as will be seen, being 1.0001755), and rearranging terms leads to

$$\frac{\rho}{\rho_f} = 1 + \alpha(c^* - c_f^*) \tag{A.7}$$

Equation A.7 can be considered the relation between ρ, ρ_f, c^*, and c_f^* as defined earlier. Experimental data published by Baxter and Wallace (1916) have been used with Equation A.2 to estimate α; Table A.1 shows the results of the computation. The differences observed in the estimates of α can be attributed to at least the temperature, the chloride concentration itself and any experimental error.

Table A.1 Determination of the Coefficient $\alpha = (\frac{\rho}{\rho_o} - 1)/c^*$

Temp. °C	ρ	ρ/ρ_o	c^* 0/00	α
0.00	1.199297	1.199455	250.82592	0.795194
	1.104825	1.104971	135.75944	0.773212
	1.043974	1.044112	57.56963	0.766234
	1.022297	1.022432	29.24018	0.767162
	1.011168	1.011301	14.71113	0.768227
	0.999868[a]	1.0	0	-
25.00	1.188510	1.192001	252.92338	0.759129
	1.096247	1.099467	136.72112	0.727520
	1.038074	1.041123	57.85477	0.710805
	1.017711	1.020701	29.35190	0.705257
	1.007470	1.010430	14.75452	0.706871
	0.997071[a]	1.0	0	-
50.04	1.176564	1.190794	255.30564	0.747316
	1.085270	1.098396	138.00811	0.712971
	1.028062	1.040496	58.37701	0.693696
	1.008124	1.020317	29.61028	0.686140
	0.998180	1.010253	14.88109	0.688963
	0.98805 [a]	1.0	0	-

[a] value of ρ_o at specified temperature (Baxter and Wallace, 1916)

Assuming that groundwater temperature is generally less than 50° C, the value of α is considered to be between 0.7 and 0.71. The estimate of α obtained from Equation A.3, using E = 0.3 and ρ_0 = 0.997071 is 0.702.

Equation A.2 can be rearranged as

$$c^* = \frac{\frac{\rho}{\rho_0} - 1}{\alpha} \tag{A.8}$$

for the expression of the chloride concentration. Table A.2 shows the values of c* obtained from Equation A.8, using different values for α while keeping the ratio $\frac{\rho}{\rho_0}$ constant. Maximum error observed (for $\Delta\alpha$ = 0.01) is 1.42 percent which has been considered negligible. The value of 0.702 for α is considered acceptable.

When the expression of the chloride concentration is derived from Equation A.7, it takes the following form:

$$c^* = c_f^* + \frac{\frac{\rho}{\rho_f} - 1}{\alpha} \tag{A.9}$$

Table A.3 shows the results of the computation of c using Equation A.9. It can be seen that while the ratio ρ/ρ_f varies, the estimates of the concentrations are not significantly affected.

Table A.2 Concentration Estimates Using Equation A.8

$\frac{\rho}{\rho_0} - 1$	α					
	0.700	0.702	0.704	0.706	0.708	0.710
0.000100	143	142	142	142	141	141
0.000200	286	285	284	283	282	282
0.000300	429	427	426	425	424	423
0.000400	571	570	568	567	565	563
0.000500	714	712	710	708	706	704
0.000600	857	855	852	850	847	845
0.000700	1,000	997	994	992	989	986
0.000800	1,143	1,140	1,136	1,133	1,130	1,127
0.000900	1,286	1,282	1,278	1,275	1,271	1,268
0.001000	1,429	1,425	1,420	1,416	1,412	1,408
0.002000	2,857	2,849	2,841	2,833	2,825	2,817
0.004000	5,714	5,698	5,682	5,666	5,650	5,634
0.006000	8,571	8,547	8,523	8,499	8,475	8,451
0.008000	11,429	11,396	11,364	11,331	11,299	11,268
0.010000	14,286	14,245	14,205	14,164	14,124	14,085
0.012000	17,143	17,094	17,045	16,997	16,949	16,901
0.014000	20,000	19,943	19,886	19,830	19,774	19,718
0.015000	21,429	21,368	21,307	21,246	21,186	21,127
0.020000	28,571	28,490	28,409	28,329	28,249	28,169
0.025000	35,714	35,613	35,511	35,411	35,311	35,211

Table A.3 Concentration Estimates Using Equation A.9 and $\alpha = 0.702$

$c_f^* = 0.0$		$c_f^* = 20$ ppm		$c_f^* = 40$ ppm	
$\frac{\rho}{\rho_f} - 1$	c^* mg/l	$\frac{\rho}{\rho_f} - 1$	c^*	$\frac{\rho}{\rho_f} - 1$	c^*
0.000100	142	0.000086	142	0.000072	142
0.000200	285	0.000186	285	0.000172	285
0.000300	427	0.000286	427	0.000272	427
0.000400	570	0.000386	570	0.000372	570
0.000500	712	0.000486	712	0.000472	712
0.000600	855	0.000586	855	0.000572	855
0.000700	997	0.000686	997	0.000672	997
0.000800	1,140	0.000786	1,140	0.000772	1,140
0.000900	1,282	0.000886	1,282	0.000872	1,282
0.001000	1,425	0.000986	1,425	0.000972	1,424
0.002000	2,849	0.001986	2,849	0.001972	2,849
0.004000	5,698	0.003986	5,698	0.003972	5,698
0.006000	8,547	0.005986	8,547	0.005972	8,547
0.008000	11,397	0.007986	11,396	0.007972	11,396
0.010000	14,245	0.009986	14,245	0.009971	14,244
0.012000	17,094	0.011986	17,094	0.011972	17,094
0.014000	19,943	0.013986	19,943	0.013972	19,943
0.015000	21,368	0.014986	21,367	0.014971	21,367
0.020000	28,490	0.019986	28,490	0.019971	28,489
0.025000	35,613	0.024986	35,612	0.024971	35,611

Table A.3--continued

$c_f^* = 80$ mg/l		$c_f^* = 140$ mg/l		$c_f^* = 240$ mg/l	
$\frac{\rho}{\rho_f} - 1$	c^* mg/l	$\frac{\rho}{\rho_f} - 1$	c^*	$\frac{\rho}{\rho_f} - 1$	c^*
0.000044	142	0.000002	143	-0.000068	143
0.000144	285	0.000102	285	0.000032	285
0.000244	427	0.000202	427	0.000132	427
0.000344	570	0.000302	570	0.000232	570
0.000444	712	0.000402	712	0.000332	712
0.000544	855	0.000502	855	0.000432	855
0.000644	997	0.000602	997	0.000532	997
0.000744	1,140	0.000702	1,140	0.000632	1,140
0.000844	1,282	0.000802	1,282	0.000732	1,282
0.000944	1,425	0.000902	1,424	0.000831	1,424
0.001944	2,849	0.001902	2,849	0.001831	2,849
0.003944	5,698	0.003902	5,698	0.003831	5,697
0.005944	8,547	0.005902	8,547	0.005831	8,546
0.007944	11,396	0.007901	11,395	0.007831	11,395
0.009943	14,244	0.009901	14,244	0.009830	14,243
0.011943	17,093	0.011901	17,093	0.011830	17,091
0.013043	19,942	0.013901	19,941	0.013829	19,940
0.14929	21,366	0.014900	21,365	0.014829	21,364
0.019928	28,488	0.019900	28,487	0.019828	28,485
0.024928	35,611	0.024899	35,609	0.024827	35,607

APPENDIX B
THE INFLUENCE FUNCTION L(η)

The vertical distribution of chloride content in underground saltwater is generally considered uniform with the ordinate c_s^*. Rubin and Pinder (1977) suggested the following relation to describe the vertical distribution of the chloride concentration in the transition zone caused by a producing well pumping from a freshwater underlain by saltwater:

$$c^* = c_s^* L(\eta) \tag{B.1}$$

where

$$L(\eta) = 1 - 2\eta + \eta^2 \tag{B.2}$$

$$\eta = \frac{Z - Z_b}{\delta} \tag{B.3}$$

$$\delta = Z_t - Z_b \tag{B.4}$$

$L(\eta)$ = the influence function describing the vertical distribution of the chloride content (in dimensionless form) in the transition zone;

c^* = chloride content at the elevation z;

c_s^* = chloride content in the underground saltwater.

Z, Z_b, Z_t, δ are defined in Figure B.1.

An elementary analysis of Equation B.2 shows that the influence function has the following characteristics:

(1) the value of $L(\eta)$ at the top of the transition zone is 0 (i.e., $L(1) = 0$);

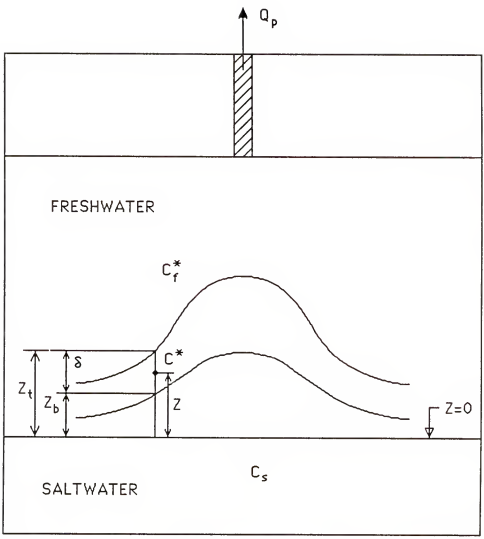


Figure B.1 The Transition Zone Between the Freshwater and the Saltwater

(2) the value of L(η) at the bottom of the transition zone is 1 (i.e., L(0) = 1);

(3) the value of the first derivative of L(η) at the top of the transition zone is 0 (i.e., L'(0) = 0).

Even though the above characteristics describe fairly well the physical behavior expected from the influence function, the actual function L(η) should also fit an experimental curve showing an actual vertical chloride distribution in coastal aquifer.

Figure B.2 (Curve A) shows a typical vertical distribution of chloride concentration in coastal aquifer. Data from the North Sea, Amsterdam, Holland (Brown, 1925); the Biscayne aquiver, Silver Bluff area, Southeastern Florida (Parker et al., 1955); and South Cross Bayou, Pineallas County, Florida (Hickey, 1982); all exhibit the same form for the vertical chloride distribution under the freshwater in coastal aquifers. The Curve A in Figure B.2 has been obtained with the assumption that the chloride content in underground saltwater is 21 g/l. Curve B on Figure B.2 shows the influence function suggested by Rubin and Pinder (1977). A rough analysis of the two curves suggests that effort should be directed toward deriving a better expression for the influence function.

In an attempt to derive an influence function which will fit the experimental Curve A of Figure B.2, a regression analysis (using points from Curve A) has been made and the results are shown in Tables B.1 through B.3 and Figures B.3 and B.4. The expression used in the regression analysis is a simple polynomial approximation in the form:

$$L(\eta) = a_0 + a_1\eta + a_2\eta^2 + a_3\eta^3 + \cdots a_n\eta^n \qquad (B.5)$$

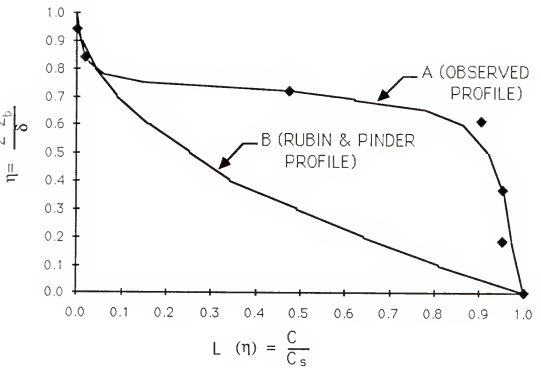


Figure B.2 Profiles of the Influence Function (η)

Table B.1 Regression Analysis of the Influence Function Using SAS Stepwise Regression Procedure

STEPWISE REGRESSION PROCEDURE FOR DEPENDENT VARIABLE Y

NOTE: SLENTRY AND SLSTAY HAVE BEEN SET TO .15 FOR THE STEPWISE TECHNIQUE

STEP 1 VARIABLE X2 ENTERED R SQUARE = 0.89545566 C(P) = 113.67852241

	DF	SUM OF SQUARES	MEAN SQUARE	F	PROB>F
REGRESSION	1	4.89721478	4.89721478	214.13	0.0001
ERROR	25	0.57174922	0.02286997		
TOTAL	26	5.46896400			

	B VALUE	STD ERROR	TYPE II SS	F	PROB>F
INTERCEPT	.00003133				
X2	.88236550	0.06029853	4.89721478	214.13	0.0001

BOUNDS ON CONDITION NUMBER: 1, 1

STEP 2 VARIABLE X8 ENTERED R SQUARE = 0.94452754 C(P) = 51.52323539

	DF	SUM OF SQUARES	MEAN SQUARE	F	PROB>F
REGRESSION	2	5.16558712	2.58279356	204.32	0.0001
ERROR	24	0.30337688	0.01264070		
TOTAL	26	5.46896400			

	B VALUE	STD ERROR	TYPE II SS	F	PROB>F
INTERCEPT	1.05309084				
X2	-1.21692638	0.08533314	2.57077662	203.37	0.0001
X8	0.17150178	0.03722077	0.26837234	21.23	0.0001

BOUNDS ON CONDITION NUMBER: 3.623401, 14.4936

Table B.1--Continued

STEPWISE REGRESSION PROCEDURE FOR DEPENDENT VARIABLE Y

STEP 3 VARIABLE X3 ENTERED R SQUARE = 0.95607718 C(P) = 38.42354233

	DF	SUM OF SQUARES	MEAN SQUARE	F	PROB>F
REGRESSION	3	5.22875168	1.74291723	166.88	0.0001
ERROR	23	0.24021233	0.01044401		
TOTAL	26	5.46896400			

	B VALUE	STD ERROR	TYPE II SS	F	PROB>F
INTERCEPT	1.00400917				
X2	0.00569592	0.50316657	0.00000134	0.00	0.9911
X3	-1.43035694	0.58162282	0.06316455	6.05	0.0219
X8	0.36744134	0.08656012	0.18819486	18.02	0.0003

BOUNDS ON CONDITION NUMBER: 263.0242, 1317.663

STEP 4 VARIABLE X2 REMOVED R SQUARE = 0.95607693 C(P) = 36.42386227

	DF	SUM OF SQUARES	MEAN SQUARE	F	PROB>F
REGRESSION	2	5.22875034	2.61437517	261.20	0.0001
ERROR	24	0.24021366	0.01000890		
TOTAL	26	5.46896400			

	B VALUE	STD ERROR	TYPE II SS	F	PROB>F
INTERCEPT	1.00426504				
X3	-1.42385158	0.08777180	2.63393983	263.16	0.0001
X8	0.36660043	0.04349975	0.71088429	71.03	0.0001

BOUNDS ON CONDITION NUMBER: 6.250344, 25.00137

Table B.1--Continued

STEPWISE REGRESSION PROCEDURE FOR DEPENDENT VARIABLE Y

STEP 5 VARIABLE X7 ENTERED R SQUARE = 0.95994207 C(P) = 33.37068892

	DF	SUM OF SQUARES	MEAN SQUARE	F	PROB>F
REGRESSION	3	5.24988861	1.74996287	183.72	0.0001
ERROR	23	0.21907539	0.00952502		
TOTAL	26	5.46896400			

	B VALUE	STD ERROR	TYPE II SS	F	PROB>F
INTERCEPT	1.01793248				
X3	-1.75330555	0.23714995	0.52063683	54.66	0.0001
X7	1.37326344	0.92183244	0.02113827	2.22	0.1499
X8	-0.66272532	0.69225877	0.00872963	0.92	0.3484

BOUNDS ON CONDITION NUMBER: 2181.648, 11678.89

STEP 6 VARIABLE X8 REMOVED R SQUARE = 0.95834585 C(P) = 33.45753611

	DF	SUM OF SQUARES	MEAN SQUARE	F	PROB>F
REGRESSION	2	5.24115898	2.62057949	276.09	0.0001
ERROR	24	0.22780502	0.00949188		
TOTAL	26	5.46896400			

	B VALUE	STD ERROR	TYPE II SS	F	PROB>F
INTERCEPT	1.00972463				
X3	-1.54659093	0.09738951	2.36935764	249.62	0.0001
X7	0.49241826	0.05640961	0.72329293	76.20	0.0001

BOUNDS ON CONDITION NUMBER: 8.197862, 32.79145

NO OTHER VARIABLES MET THE 0.1500 SIGNIFICANCE LEVEL FOR ENTRY INTO THE MODEL

Table B.1--Continued

SUMMARY OF STEPWISE REGRESSION PROCEDURE FOR DEPENDENT VARIABLE Y

STEP	VARIABLE ENTERED	VARIABLE REMOVED	NUMBER IN	PARTIAL R**2	MODEL R**2	C(P)	F	PROB>F
1	X2		1	0.8955	0.8955	113.679	214.1330	0.0001
2	X8		2	0.0491	0.9445	51.523	21.2308	0.0001
3	X3		3	0.0115	0.9561	38.424	6.0479	0.0219
4		X2	2	0.0000	0.9561	36.424	0.0001	0.9911
5	X7		3	0.0039	0.9599	33.371	2.2192	0.1499
6		X8	2	0.0016	0.9583	33.458	0.9165	0.3484

Table B.2 Coefficient of the Influence Function Using

$$L(n) = a_0 + a_2 n^2 + a_3 n^3 + a_8 n^8$$

DEP VARIABLE: Y

ANALYSIS OF VARIANCE

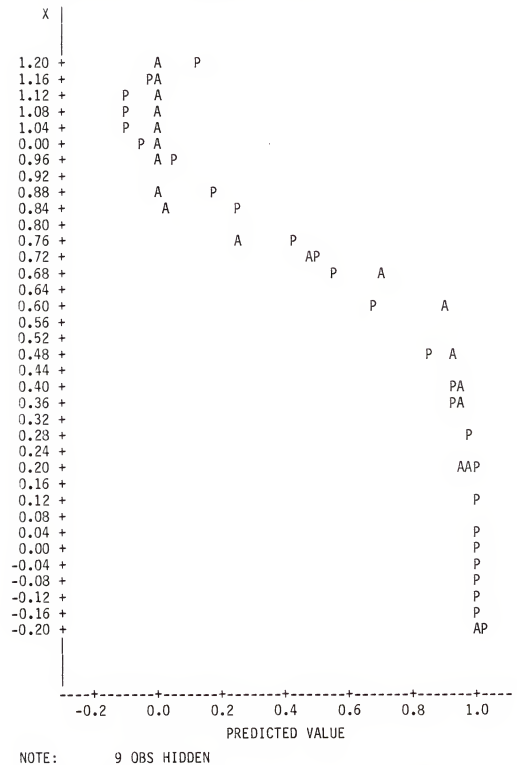
SOURCE	DF	SUM OF SQUARES	MEAN SQUARE	F VALUE	PROB>F
MODEL	2	5.228617	2.614308	261.053	0.0001
ERROR	24	0.2403474	0.01001448		
C TOTAL	26	5.468964			

ROOT MSE	0.1000724	R-SQUARE	0.9561
DEP MEAN	0.5960731	ADJ R-SQ	0.9524
C.V.	16.7886		

PARAMETER ESTIMATES

VARIABLE	DF	PARAMETER ESTIMATE	STANDARD ERROR	T FOR HO: PARAMETER=0
INTERCEP	1	1	1.86399E-10	99999.999
X2	1	0.04238747	0.3780993	0.112
X3	1	-1.46781	0.4694702	-3.127
X8	1	0.3714289	0.0774965	4.793
RESTRICT	-1	0.03369407	0.2901106	0.116

VARIABLE	DF	PROB > |T|
INTERCEP	1	0.0001
X2	1	0.9117
X3	1	0.0046
X8	1	0.0001
RESTRICT	-1	0.9085



NOTE: 9 OBS HIDDEN

Figure B.3 Approximation of the Influence Function Using $L(\eta) = a_0 + a_2\eta^2 + a_3\eta^3 + a_8\eta^8$

Table B.3 Coefficient of the Influence Function Using $L(\eta) = a_0 + a_3\eta^3 + a_7\eta^7 + a_8\eta^8$

DEP VARIABLE: Y

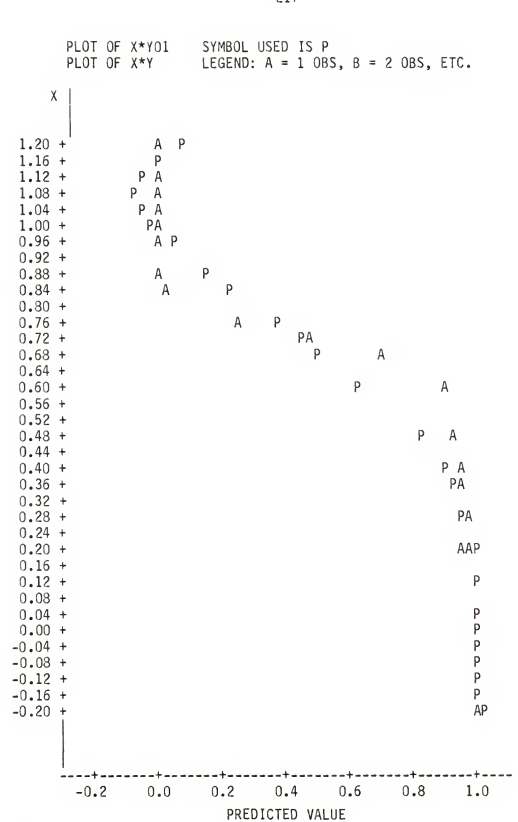
ANALYSIS OF VARIANCE

SOURCE	DF	SUM OF SQUARES	MEAN SQUARE	F VALUE	PROB>F
MODEL	2	5.245813	2.622907	282.095	0.0001
ERROR	24	0.2231508	0.009297949		
C TOTAL	26	5.468964			

ROOT MSE	0.09642587	R-SQUARE	0.9592
DEP MEAN	0.5960731	ADJ R-SQ	0.9553
C.V.	16.17685		

PARAMETER ESTIMATES

VARIABLE	DF	PARAMETER ESTIMATE	STANDARD ERROR	T FOR HO: PARAMETER=0	PROB > |T|
INTERCEP	1	1	.	.	.
X3	1	-1.67484	0.2021176	-8.286	0.0001
X7	1	1.171473	0.8582638	1.365	0.1849
X8	1	-0.521115	0.6496507	-0.802	0.4303
RESTRICT	-1	0.2272627	0.3432713	0.662	0.5142



NOTE: 9 OBS HIDDEN

Figure B.4 Approximation of the Influence Function Using $L(n) = a_0 + a_3 n^3 + a_7 n^7 + a_8 n^8$

The stepwise regression analysis, using n=8 (Table B.1) suggests two possible expressions in the form

$$L_1(\eta) = 1 + 0.0424\ \eta^2 - 1.4678\ \eta^3 + 0.3714\ \eta^8 \qquad (B.6)$$

$$L_2(\eta) = 1 - 1.67484\ \eta^3 + 1.171473\ \eta^7 - 0.52111\ \eta^8 \qquad (B.7)$$

The evaluation of the first derivative of those two expressions at the bottom of the transition zone (η=0) yields zero. However, in order for the salt to disperse from the saltwater zone into the transition zone, the gradient $\frac{\partial c^*}{\partial z}$ and consequently $\frac{\partial L(\eta)}{\partial \eta}$ can not be zero at Z_b. Therefore, none of those two expressions can effectively represent the influence function. On the other hand, the chloride concentration in the standard saltwater is 35 g/l (see Appendix A), while the value of the chloride content in underground saltwater and reported in groundwater literature (Brown, 1925; Parker et al., 1955; Hickey, 1982) varies from 17 g/l to 21 g/l. This suggests that most of the considered underground saltwater is actually from the transition zone, since, by definition the transition zone is the region of the underground water where the chloride content varies from that of the saltwater (35 g/l) to that of the freshwater. A possible way of solving that conflicting situation would be to define a standard chloride content for underground saltwater. For the purpose of this discussion, the following has been assumed:

> A groundwater with more than 19 g/l of chloride is an underground saltwater.

With that definition, the chloride distribution in underground saltwater is not necessary uniform any longer. Therefore, a function describing the vertical profile in underground saltwater would also be in order.

However that analysis is beyond the scope of the present work. It will be suggested in the recommendations for future work.

In the present study, the influence function suggested by Rubin and Pinder (1977) will be used in conjunction with 19 g/l as the underground chloride concentration.

APPENDIX C
INTEGRATION OF THE TRANSPORT AND FLOW EQUATIONS
USING LEIBNITZ'S RULE

C.1 Expression of Leibnitz's Rule

According to Korn and Korn (1961), Leibnitz's rule states:

$$\frac{\partial}{\partial\lambda}\int_{u(\lambda)}^{v(\lambda)} f(x,\lambda)\,dx = \int_{u(\lambda)}^{v(\lambda)} \frac{\partial}{\partial\lambda} f(x,\lambda)\,dx + f(v,\lambda)\frac{\partial v}{\partial\lambda} - f(u,\lambda)\frac{\partial u}{\partial\lambda} \quad (C.1)$$

therefore,

$$\int_{u(\lambda)}^{v(\lambda)} \frac{\partial}{\partial\lambda} f(x,\lambda)\,dx = \frac{\partial}{\partial\lambda}\int_{u(\lambda)}^{v(\lambda)} f(x,\lambda)\,dx - f(v,\lambda)\frac{\partial v}{\partial\lambda} + f(u,\lambda)\frac{\partial u}{\partial x} \quad (C.2)$$

C.2 Integration of the Transport Equation

The transport equation as expressed by Equation 4.71 is

$$\begin{aligned} n\frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) - \left(\frac{c}{c_s}\right) S_o \frac{\partial s}{\partial t} &= \frac{\partial}{\partial x} D_{xx}\frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial x} D_{xy}\frac{\partial}{\partial y}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial x} D_{xz}\frac{\partial}{\partial z}\left(\frac{c}{c_s}\right) \\ &+ \frac{\partial}{\partial y} D_{yx}\frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial y} D_{yy}\frac{\partial}{\partial y}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial y} D_{yz}\frac{\partial}{\partial z}\left(\frac{c}{c_s}\right) \\ &+ \frac{\partial}{\partial z} D_{zx}\frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial z} D_{zy}\frac{\partial}{\partial y}\left(\frac{c}{c_s}\right) + \frac{\partial}{\partial z} D_{zz}\frac{\partial}{\partial z}\left(\frac{c}{c_s}\right) \\ &- \frac{\partial}{\partial x}\left[q_x \frac{c}{c_s}\right] - \frac{\partial}{\partial y}\left[q_y \frac{c}{c_s}\right] - \frac{\partial}{\partial z}\left[q_z \frac{c}{c_s}\right] \\ &+ \left\{\begin{matrix}\text{source}\\ \text{rates}\end{matrix}\right) - \left\{\begin{matrix}\text{sink}\\ \text{rates}\end{matrix}\right) \end{aligned} \quad (C.3)$$

where

1) for $Z_o \leq Z < Z_b$

$$\frac{c}{c_s} = 1 \tag{C.4}$$

$$\frac{\partial}{\partial z}\left(\frac{c}{c_s}\right) = 0 \tag{C.5}$$

2) for $Z_b \leq Z \leq Z_t$

$$\frac{c}{c_s} = L(\eta) \tag{C.6}$$

$$\frac{\partial}{\partial z}\left(\frac{c}{c_s}\right) = \frac{\partial L(\eta)}{\partial \eta} \cdot \frac{\partial \eta}{\partial z}$$

or

$$\frac{\partial}{\partial z}\left(\frac{c}{c_s}\right) = L'(\eta) \cdot \frac{\partial \eta}{\partial z} \tag{C.7}$$

and since

$$\eta = \frac{Z - Z_b}{\delta}$$

$$\frac{\partial \eta}{\partial z} = \frac{1}{\delta} \tag{C.8}$$

Therefore

$$\frac{\partial}{\partial z}\left(\frac{c}{c_s}\right) = \frac{L'(\eta)}{\delta} \tag{C.9}$$

3) for $Z_t < Z$

$$\frac{c}{c_s} = 0 \tag{C.10}$$

$$\frac{\partial}{\partial z}\left(\frac{c}{c_s}\right) = 0 \tag{C.11}$$

The integration of Equation C.3 from Z_o to Z_L can be written as

$$\int_{Z_o}^{Z_L} (C.3)\, dz = \int_{Z_o}^{Z_b} (C.3)\, dz + \int_{Z_b}^{Z_t} (C.3)\, dz + \int_{Z_t}^{Z_L} (C.3)\, dz \tag{C.12}$$

Considering Equations C.6 through C.11, when

1) $Z_t < Z_L$

$$\int_{Z_t}^{Z_L} (C.3)\, dz = 0 \qquad (C.13)$$

2) $Z_t > Z_L$

$$\int_{Z_t}^{Z_L} (C.3)\, dz = -\int_{Z_L}^{Z_t} (C.3)\, dz \qquad (C.14)$$

It should also be noted that the horizontal specific discharges q_x and q_y implicitly have vertically averaged values and, therefore, are not functions of z. Using the mean value of the vertical specific discharge q_z in the computation ofthe dispersion coefficients (Equation 4.24) the latter will not be a function of z either.

In order to facilitate the discussion, instead of integrating the whole Equation C.3 as shown in Equation C.12, the terms of Equation C.3 will be integrated individually.

C.2.1 Integration of $n\frac{\partial}{\partial t}\left(\frac{c}{c_s}\right)$

$$\int_{Z_o}^{Z_b} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz = n\left\{\frac{\partial}{\partial t}\int_{Z_o}^{Z_b}\left(\frac{c}{c_s}\right)dz - \frac{c}{c_s}\Big|_{Z_b}\frac{\partial Z_b}{\partial t} + \frac{c}{c_s}\Big|_{Z_o}\frac{\partial Z_o}{\partial t}\right. \qquad (C.15)$$

since $\frac{c}{c_s}\Big|_{Z_b} = 1$ and $\frac{\partial Z_o}{\partial t} = 0$, Equation C.15 becomes

$$\int_{Z_o}^{Z_b} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right)dz = n\left\{\frac{\partial Z_b}{\partial t} - \frac{\partial Z_b}{\partial t}\right\}$$

Therefore

$$\int_{Z_o}^{Z_b} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz = 0 \qquad (C.16)$$

and

$$\int_{Z_b}^{Z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz = n\left\{\frac{\partial}{\partial t}\int_{Z_b}^{Z_t}\left(\frac{c}{c_s}\right) dz - \frac{c}{c_s}\Big|_{Z_t}\frac{\partial Z_t}{\partial t} + \frac{c}{c_s}\Big|_{Z_b}\frac{\partial Z_b}{\partial t}\right\} \qquad (C.17)$$

since $\left.\frac{c}{c_s}\right|_{Z_t} = 0$

$$\int_{Z_b}^{Z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz = n\left\{\frac{\partial}{\partial t}\delta\int_0^1 L(\eta)d\eta + \frac{\partial Z_b}{\partial t}\right\} \qquad (C.18)$$

Finally,

for $Z_b < Z_L < Z_t$,

$$\int_{Z_L}^{Z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz = n \frac{\partial}{\partial t}\left(\delta\int_{\eta_L}^{1} L(\eta)d\eta\right) \qquad (C.19a)$$

for $Z_b > Z_L$,

$$\int_{Z_L}^{Z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz = n\left\{\frac{\partial}{\partial t}\left[Z_b + \delta\int_0^1 L(\eta)d\eta\right]\right\} \qquad (C.19b)$$

By making use of the fact that

$$\int_{Z_b}^{Z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz = \int_{Z_b}^{Z_L} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz + \int_{Z_L}^{Z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz \qquad (C.20)$$

and

$$\int_{Z_b}^{Z_L} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz = \int_{Z_b}^{Z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz - \int_{Z_L}^{Z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz \qquad (C.21)$$

when $Z_t > Z_L$, only $\int_{Z_b}^{Z_t} n\frac{\partial}{\partial t}(\frac{c}{c_s})dz$ will be considered; Equation C.21 will be used, in the specific case when $Z_t > Z_L$, to determine $\int_{Z_b}^{Z_L} n\frac{\partial}{\partial t}(\frac{c}{c_s})dz$. In other words, Equation C.3 will be integrated from Z_o to Z_t and the term $\int_{Z_L}^{Z_t} n\frac{\partial}{\partial t}(\frac{c}{c_s})dz$ will be considered as a sink term which is zero when $Z_t < Z_L$ and non-zero when $Z_t > Z_L$. This approach is relevant since the position of Z_t is not know before the computation of C.3 is completed. Hereafter, the integration of the remaining terms will be done from Z_o to Z_b and from Z_b to Z_t only.

C.2.2 Integration of $(\frac{c}{c_s})\, S_o \frac{\partial s}{\partial t}$

Since $S_o \frac{\partial s}{\partial t}$ is independent of Z within the limits Z_o, Z_L,

$$\int_{Z_o}^{Z_b} (\frac{c}{c_s})\, S_o \frac{\partial s}{\partial t}\, dZ = Z_b\, S_o \frac{\partial s}{\partial t} \qquad (C.22)$$

and

$$\int_{Z_b}^{Z_t} (\frac{c}{c_s})\, S_o \frac{\partial s}{\partial t}\, dz = (\delta \int_0^1 L(n)dn)\, S_o \frac{\partial s}{\partial t} \qquad (C.23)$$

C.2.3 Integration of $\frac{\partial}{\partial x} D_{xx} \frac{\partial}{\partial x}(\frac{c}{c_s})$, $\frac{\partial}{\partial x} D_{xy} \frac{\partial}{\partial y}(\frac{c}{c_s})$, $\frac{\partial}{\partial y} D_{yx} \frac{\partial}{\partial x}(\frac{c}{c_s})$, and $\frac{\partial}{\partial y} D_{yy} \frac{\partial}{\partial y}(\frac{c}{c_s})$

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial x} D_{xx} \frac{\partial}{\partial x}(\frac{c}{c_s})\, dz = \frac{\partial}{\partial x}\{D_{xx} \int_{Z_o}^{Z_b} \frac{\partial}{\partial x}(\frac{c}{c_s})\, dz\} - [D_{xx} \frac{\partial}{\partial x}(\frac{c}{c_s})]\Big|_{Z_b} \frac{\partial Z_b}{\partial x}$$

$$+ [D_{xx} \frac{\partial}{\partial x}(\frac{c}{c_s})]\Big|_{Z_o} \frac{\partial Z_o}{\partial x} \qquad (C.24)$$

The value of $\frac{\partial}{\partial x}\left(\frac{c}{c_s}\right)\Big|_{Z_o}$ is zero and assuming that $\frac{\partial}{\partial x}\left(\frac{c}{c_s}\right)\Big|_{Z_b} \approx 0$, Equation C.24 becomes

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial x} D_{xx} \frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) dz = 0 \qquad (C.25)$$

By analogy, the following terms are evaluated:

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial x} D_{xy} \frac{\partial}{\partial y}\left(\frac{c}{c_s}\right) dz = 0 \qquad (C.26)$$

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial y} D_{yx} \frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) dz = 0 \qquad (C.27)$$

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial y} D_{yy} \frac{\partial}{\partial y}\left(\frac{c}{c_s}\right) dz = 0 \qquad (C.28)$$

On another hand,

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial x} D_{xx} \frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) dz = \frac{\partial}{\partial x}\int_{Z_b}^{Z_t} D_{xx} \frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) dz - D_{xx} \frac{\partial}{\partial x}\left(\frac{c}{c_s}\right)\Big|_{Z_t} \frac{\partial Z_t}{\partial x}$$

$$+ D_{xx} \frac{\partial}{\partial x}\left(\frac{c}{c_s}\right)\Big|_{Z_b} \frac{\partial Z_b}{\partial x} \qquad (C.29)$$

which, also by assuming that $\frac{\partial}{\partial x}\left(\frac{c}{c_s}\right)\Big|_{Z_t} \approx 0$, simplifying, and expanding the remaining term on the right hand side, (i.e., $[\frac{\partial}{\partial x}\int_{Z_b}^{Z_t} D_{xx}\frac{\partial}{\partial x}(\frac{c}{c_s})dz]$), becomes:

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial x} D_{xx} \frac{\partial}{\partial x} \left(\frac{c}{c_s}\right) dz = \frac{\partial}{\partial x} \{D_{xx} [\frac{\partial}{\partial x} \int_{Z_b}^{Z_t} \left(\frac{c}{c_s}\right) dz - \frac{c}{c_s}\Big|_{Z_t} \frac{\partial Z_t}{\partial x}$$

$$+ \frac{c}{c_s}\Big|_{Z_b} \frac{\partial Z_b}{\partial x}]\} \qquad (C.30)$$

and since

$$\int_{Z_b}^{Z_t} \left(\frac{c}{c_s}\right) dz = \delta \int_0^1 L(\eta)\, d\eta$$

$$\frac{c}{c_s}\Big|_{Z_t} = 0$$

$$\frac{c}{c_s}\Big|_{Z_b} = 1$$

Equation C.29 finally takes the form

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial x} D_{xx} \frac{\partial}{\partial x} \left(\frac{c}{c_s}\right) dz = \frac{\partial}{\partial x} D_{xx} \frac{\partial}{\partial x} (\delta \int_0^1 L(\eta)\, d\eta) + \frac{\partial}{\partial x} D_{xx} \frac{\partial}{\partial x} (Z_b) \qquad (C.31)$$

Again, by analogy, one can write

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial x} D_{xy} \frac{\partial}{\partial y} \left(\frac{c}{c_s}\right) dz = \frac{\partial}{\partial x} D_{xy} \frac{\partial}{\partial y} (\delta \int_0^1 L(\eta)\, d\eta) + \frac{\partial}{\partial x} D_{xy} \frac{\partial}{\partial y} (Z_b) \qquad (C.32)$$

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial y} D_{yx} \frac{\partial}{\partial x} \left(\frac{c}{c_s}\right) dz = \frac{\partial}{\partial y} D_{yx} \frac{\partial}{\partial x} (\delta \int_0^1 L(\eta)\, d\eta) + \frac{\partial}{\partial y} D_{yx} \frac{\partial}{\partial x} (Z_b) \qquad (C.33)$$

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial y} D_{yy} \frac{\partial}{\partial y} \left(\frac{c}{c_s}\right) dz = \frac{\partial}{\partial y} D_{yy} \frac{\partial}{\partial y} (\delta \int_0^1 L(\eta)\, d\eta) + \frac{\partial}{\partial y} D_{yy} \frac{\partial}{\partial y} (Z_b) \qquad (C.34)$$

C.2.4 Integration of $\frac{\partial}{\partial x} D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right)$ and $\frac{\partial}{\partial y} D_{yz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right)$

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial x} D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) dz = \frac{\partial}{\partial x} \int_{Z_o}^{Z_b} D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) dz - D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right)\Big|_{Z_b} \frac{\partial Z_b}{\partial x} + D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right)\Big|_{Z_o} \frac{\partial Z_o}{\partial x} \qquad (C.35)$$

and since

$$\frac{\partial}{\partial z} \left(\frac{c}{c_s}\right)\Big|_{Z_o} = 0$$

$$\frac{\partial}{\partial z} \left(\frac{c}{c_s}\right)\Big|_{Z_b} = \frac{L'(0)}{\delta}$$

Equation C.35 becomes

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial x} D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) dz = \frac{\partial}{\partial x} \left\{D_{xz}\left[\frac{c}{c_s}\Big|_{Z_b} - \frac{c}{c_s}\Big|_{Z_o}\right]\right\} - D_{xz} \frac{L'(0)}{\delta} \frac{\partial Z_b}{\partial x}$$

or

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial x} D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) dz = - D_{xz} \frac{L'(0)}{\delta} \frac{\partial Z_b}{\partial x} \qquad (C.36)$$

and by analogy

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial y} D_{yz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) dz = - D_{yz} \frac{L'(0)}{\delta} \frac{\partial Z_b}{\partial y} \qquad (C.37)$$

On another hand,

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial x} D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) dz = \frac{\partial}{\partial x} \int_{Z_b}^{Z_t} D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) dz - D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right)\Big|_{Z_t} \frac{\partial Z_t}{\partial x} + D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right)\Big|_{Z_b} \frac{\partial Z_b}{\partial x}$$

or

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial x} D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) dz = \frac{\partial}{\partial x} \left\{D_{xz} \left[\frac{c}{c_s}\Big|_{Z_t} - \frac{c}{c_s}\Big|_{Z_b}\right]\right\}$$

$$- D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right)\Big|_{Z_t} \frac{\partial Z_t}{\partial x} + D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right)\Big|_{Z_b} \frac{\partial Z_b}{\partial x} \qquad (C.38)$$

Introducing Equations C.6 and C.9 into C.38 yields

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial x} D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) dz = \frac{\partial}{\partial x} \left[D_{xz} \left(L(1) - L(0)\right)\right]$$

$$- D_{xz} \left(\frac{\partial Z_t}{\partial x}\right)\left(\frac{L'(1)}{\delta}\right) + D_{xz} \left(\frac{\partial Z_b}{\partial x}\right)\left(\frac{L'(0)}{\delta}\right) \qquad (C.39)$$

and since $L(1) = 0$, $L(0) = 1$, and $L'(1) = 0$, Equation C.39 becomes

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial x} D_{xz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) dz = - \frac{\partial}{\partial x} \left(D_{xz}\right) + D_{xz} \frac{L'(0)}{\delta} \frac{\partial}{\partial x} \left(Z_b\right) \qquad (C.40)$$

and by analogy

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial y} D_{yz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) dz = - \frac{\partial}{\partial y} \left(D_{yz}\right) + D_{yz} \frac{L'(0)}{\delta} \frac{\partial}{\partial y} \left(Z_b\right) \qquad (C.41)$$

C.2.5 Integration of $\frac{\partial}{\partial z} D_{zx} \frac{\partial}{\partial x} \left(\frac{c}{c_s}\right)$ and $\frac{\partial}{\partial z} D_{zy} \frac{\partial}{\partial y} \left(\frac{c}{c_s}\right)$

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial z} D_{zx} \frac{\partial}{\partial x} \left(\frac{c}{c_s}\right) dz = D_{zx} \left\{\frac{\partial}{\partial x} \left(\frac{c}{c_s}\right)\Big|_{Z_b} - \frac{\partial}{\partial x} \left(\frac{c}{c_s}\right)\Big|_{Z_o}\right\} \qquad (C.42)$$

and

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial z} D_{zx} \frac{\partial}{\partial x} \left(\frac{c}{c_s}\right) dz = D_{zx} \left\{\frac{\partial}{\partial x} \left(\frac{c}{c_s}\right)\Big|_{Z_t} - \frac{\partial}{\partial x} \left(\frac{c}{c_s}\right)\Big|_{Z_b}\right\} \qquad (C.43)$$

Considering the previous assumptions stating that

$$\frac{\partial}{\partial x}\left(\frac{c}{c_s}\right)\Big|_{Z_o} = 0$$

$$\frac{\partial}{\partial x}\left(\frac{c}{c_s}\right)\Big|_{Z_b} \approx 0$$

$$\frac{\partial}{\partial x}\left(\frac{c}{c_s}\right)\Big|_{Z_t} \approx 0$$

Equations C.42 and C.43 become, respectively,

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial z} D_{zx} \frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) dz = 0 \qquad (C.44)$$

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial z} D_{zx} \frac{\partial}{\partial x}\left(\frac{c}{c_s}\right) dz = 0 \qquad (C.45)$$

and by analogy,

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial z} D_{zy} \frac{\partial}{\partial y}\left(\frac{c}{c_s}\right) dz = 0 \qquad (C.46)$$

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial z} D_{zy} \frac{\partial}{\partial y}\left(\frac{c}{c_s}\right) dz = 0 \qquad (C.47)$$

C.2.6 Integration of $\frac{\partial}{\partial z} D_{zz} \frac{\partial}{\partial z}\left(\frac{c}{c_s}\right)$

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial z} D_{zz} \frac{\partial}{\partial z}\left(\frac{c}{c_s}\right) dz = D_{zz}\left\{\frac{\partial}{\partial z}\left(\frac{c}{c_s}\right)\Big|_{Z_b} - \frac{\partial}{\partial z}\left(\frac{c}{c_s}\right)\Big|_{Z_o}\right\} \qquad (C.48)$$

Substitution of Equations C.5 and C.9 into Equation C.48 yields

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial z} D_{zz} \frac{\partial}{\partial z}\left(\frac{c}{c_s}\right) dz = D_{zz} \frac{L'(0)}{\delta} \qquad (C.49)$$

On the other hand,

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial z} D_{zz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) dz = D_{zz} \left\{ \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) \Big|_{Z_t} - \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) \Big|_{Z_b} \right\} \tag{C.50}$$

and the introduction of Equation C.9 into Equation C.50 leads to

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial z} D_{zz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) dz = D_{zz} \left\{ \frac{L'(1)}{\delta} - \frac{L'(0)}{\delta} \right\} \tag{C.51}$$

and since $L'(1) = 0$, Equation C.51 becomes

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial z} D_{zz} \frac{\partial}{\partial z} \left(\frac{c}{c_s}\right) dz = -D_{zz} \left(\frac{L'(0)}{\delta}\right) \tag{C.52}$$

C.2.7 Integration of $\frac{\partial}{\partial x}\left[q_x \frac{c}{c_s}\right]$ and $\frac{\partial}{\partial y}\left[q_y \frac{c}{c_s}\right]$

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial x} \left[q_x \frac{c}{c_s}\right] dz = \frac{\partial}{\partial x} \int_{Z_o}^{Z_b} q_x \frac{c}{c_s} dz - \left(q_x \frac{c}{c_s}\right)\Big|_{Z_b} \frac{\partial Z_b}{\partial x} + \left(q_x \frac{c}{c_s}\right)\Big|_{Z_o} \frac{\partial Z_o}{\partial x} \tag{C.53}$$

which reduces to

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial x} \left[q_x \frac{c}{c_s}\right] dz = \frac{\partial}{\partial x} \left[q_x Z_b\right] - q_x \frac{\partial Z_b}{\partial x}$$

or

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial x} \left[q_x \frac{c}{c_s}\right] dz = Z_b \frac{\partial}{\partial x} q_x \tag{C.54}$$

and, by analogy

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial y} \left[q_y \frac{c}{c_s}\right] dz = Z_b \frac{\partial}{\partial y} q_y \tag{C.55}$$

on the other hand,

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial x}\left[q_x \frac{c}{c_s}\right] dz = \frac{\partial}{\partial x}\int_{Z_b}^{Z_t} q_x \frac{c}{c_s}\, dz - q_x \frac{c}{c_s}\Big|_{Z_t} \frac{\partial Z_t}{\partial x} + q_x \frac{c}{c_s}\Big|_{Z_b} \frac{\partial Z_b}{\partial x} \tag{C.56}$$

which reduces to

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial x}\left[q_x \frac{c}{c_s}\right] dz = \frac{\partial}{\partial x} q_x \left(\delta \int_0^1 L(\eta)\, d\eta\right) + q_x \frac{\partial Z_b}{\partial x} \tag{C.57}$$

and similarly

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial y}\left[q_y \frac{c}{c_s}\right] dz = \frac{\partial}{\partial y} q_y \left(\delta \int_0^1 L(\eta)\, d\eta\right) + q_y \frac{\partial Z_b}{\partial y} \tag{C.58}$$

C.2.8 Integration of $\frac{\partial}{\partial z}\left[q_z \frac{c}{c_s}\right]$

It is obvious that

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial z}\left[q_z \frac{c}{c_s}\right] dz = \left(q_z \frac{c}{c_s}\right)\Big|_{Z_b} - \left(q_z \frac{c}{c_s}\right)\Big|_{Z_o} \tag{C.59}$$

and

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial z}\left[q_z \frac{c}{c_s}\right] dz = \left(q_z \frac{c}{c_s}\right)\Big|_{Z_t} - \left(q_z \frac{c}{c_s}\right)\Big|_{Z_b} \tag{C.60}$$

Defining

$$q_{z_o} = q_z\Big|_{z_o} \tag{C.61}$$

$$q_{z_b} = q_z\Big|_{z_b} = nV_z\Big|_{z_b} = nV_{z_b} \tag{C.62}$$

$$q_{z_t} = q_z\Big|_{z_t} = nV_z\Big|_{z_t} = nV_{z_t} \tag{C.63}$$

where

V_z = pore velocity,

it is obvious that

$$V_{z_b} = n \frac{\partial Z_b}{\partial t} \tag{C.64}$$

$$V_{z_t} = n \frac{\partial Z_b}{\partial t} \tag{C.65}$$

since

$$\frac{c}{c_s}\Big|_{z_o} = \frac{c}{c_s}\Big|_{z_b} = 1$$

Equation C.59 becomes

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial z}\left[q_z \frac{c}{c_s}\right] dz = n \frac{\partial Z_b}{\partial t} - q_{z_o} \tag{C.66}$$

and since

$$\frac{c}{c_s}\Big|_{z_t} = 0$$

Equation C.60 reduces to

$$\int_{Z_b}^{Z_t} \frac{\partial}{\partial z}\left[q_z \frac{c}{c_s}\right] dz = -n \frac{\partial Z_b}{\partial t} \tag{C.67}$$

C.2.9 Determination of $\frac{c}{c_s}$

It is important to notice that the integration of the terms of Equation C.3 reveals consistently three terms Z_b, $\delta\int_0^{\eta_L} L(n)dn$, and $\delta\int_0^1 L(n)dn$. Evidently, those terms should be related to the determination of $\frac{c}{c_s}$ in the lower zone. In order to find how $\frac{c}{c_s}$, Z_b,

$\delta\int_0^{\eta_L} L(\eta)d\eta$, and $\delta\int_0^1 L(\eta)d\eta$ are related, the following integration should be carried out:

$$Z_L\left(\overline{\frac{c}{c_s}}\right) = \int_{Z_o}^{Z_L} \frac{c}{c_s}\,dz = \int_{Z_o}^{Z_b} \frac{c}{c_s}\,dz + \int_{Z_b}^{Z_t} \frac{c}{c_s}\,dz - \int_{Z_L}^{Z_t} \frac{c}{c_s}\,dz \qquad (C.68)$$

when $Z_b > Z_L$, $\frac{c}{c_s}$ in the lower zone is constant and equal to 1.

When $Z_b < Z_L < Z_t$, Equation C.68 leads to

$$Z_L\left(\overline{\frac{c}{c_s}}\right) = Z_b + \delta\int_0^1 L(\eta)d\eta - \delta\int_{\eta_L}^1 L(\eta)d\eta \qquad (C.69)$$

or

$$\left(\overline{\frac{c}{c_s}}\right) = \frac{Z_b + \delta\int_0^1 L(\eta)d\eta}{Z_L} - \frac{\delta}{Z_L}\int_{\eta_L}^1 L(\eta)d\eta \qquad (C.70)$$

but, when $Z_t < Z_L$,

$$\int_{\eta_L}^1 L(\eta)d\eta = 0 \qquad (C.71)$$

Thus, instead of seeking the determination of $\frac{c}{c_s}$ in the lower zone, Z_b and δ are the parameters to be sought. The integration of Equation C.3 should therefore be rearranged in such a way that Z_b and δ can be determined and $\frac{c}{c_s}$ is then defined by Equation C.70. Referring back to Equation C.3, it is obvious that the source term is zero while the sink term is represented in Equation C.21 by $\int_{Z_L}^{Z_t} n\frac{\partial}{\partial t}\left(\frac{c}{c_s}\right)dz$.

It should be pointed out that the sink term in the transport equation for the lower zone becomes a source term in the transport

equation for the pumpage zone. A close look at the transport equation for the pumpage zone (Equation 4.69) shows that the source term in the pumpage zone and related to the lower zone is $\frac{1}{BP}\frac{c}{c_s}\Big|_{Z_L} q_{z_L}$ (from the advective term $\frac{\partial}{\partial z}\left[\frac{c}{c_s} q_z\right]$). This is due in part to the assumption of no dispersion in the pumpage zone, so that the source term obtained comes from the advective term only. On the other hand, the integration of Equation C.3 from Z_o to Z_t gives

$$\int_{Z_o}^{Z_b} \frac{\partial}{\partial z}\left[q_z \frac{c}{c_s}\right] dz = -q_{z_o} \tag{C.72}$$

from the combination of C.66 and C.67. This hides the advective term at Z_L. From the analysis of Equations C.12 and C.19, it is obvious that the source term in the pumpage zone should be replaced by

$$\frac{1}{BP}\int_{Z_L}^{Z_t} n \frac{\partial}{\partial t}\left(\frac{c}{c_s}\right) dz,$$

the integral being evaluated by Expressions C.19a and C.19b.

The rearrangement of the integration of Equation C.3 should lead to two equations since two parameters, Z_b and δ, are to be determined. This is done by considering a first integration of C.3 from Z_o to Z_b and a second one from Z_b to Z_t, which leads to

$$n\frac{\partial Z_b}{\partial t} + Z_b\left[\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} - S_o\frac{\partial s}{\partial t}\right] = q_{z_o} - \frac{L'(0)}{\delta}\left(D_{xz}\frac{\partial Z_b}{\partial x} + D_{yz}\frac{\partial Z_b}{\partial y} - D_{zz}\right), \tag{C.73}$$

and

$$n \frac{\partial}{\partial t}\left(\delta \int_0^1 L(\eta)d\eta\right) - \left(\delta \int_0^1 L(\eta)d\eta\right) S_o \frac{\partial s}{\partial t} = \frac{\partial}{\partial x} D_{xx} \frac{\partial}{\partial x}\left(\delta \int_0^1 L(\eta)d\eta\right)$$

$$+ \frac{\partial}{\partial x} D_{xx} \frac{\partial Z_b}{\partial x} + \frac{\partial}{\partial x} D_{xy} \frac{\partial}{\partial y}\left(\delta \int_0^1 L(\eta)d\eta\right) + \frac{\partial}{\partial x} D_{xy} \frac{\partial Z_b}{\partial y}$$

$$- \frac{\partial}{\partial x} D_{xz} + D_{xz} \frac{L'(0)}{\delta} \frac{\partial Z_b}{\partial x} + \frac{\partial}{\partial y} D_{yx} \frac{\partial}{\partial x}\left(\delta \int_0^1 L(\eta)d\eta\right)$$

$$+ \frac{\partial}{\partial y} D_{yx} \frac{\partial Z_b}{\partial x} + \frac{\partial}{\partial y} D_{yy} \frac{\partial}{\partial y}\left(\delta \int_0^1 L(\eta)d\eta\right) + \frac{\partial}{\partial y} D_{yy} \frac{\partial Z_b}{\partial y}$$

$$- \frac{\partial}{\partial y} D_{yz} + D_{yz} \frac{L'(0)}{\delta} \frac{\partial Z_b}{\partial y} - D_{zz} \frac{L'(0)}{\delta}$$

$$- \frac{\partial}{\partial x}\left[q_x \delta \int_0^1 L(\eta)d\eta\right] - q_x \frac{\partial Z_b}{\partial x} - \frac{\partial}{\partial y}\left[q_y \delta \int_0^1 L(\eta)d\eta\right] - q_y \frac{\partial Z_b}{\partial y} \qquad (C.74)$$

and

$$\frac{c}{c_s} = \frac{Z_b + \delta \int_o^{n_L} L(\eta)d\eta}{Z_L} \qquad (C.75)$$

Equations C.73, C.74 and C.75 together represent the transport equation for the lower zone.

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I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a dissertation for the degree of Doctor of Philosophy.

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